

Communication-Avoiding Algorithms for Linear Algebra and Beyond

Jim Demmel

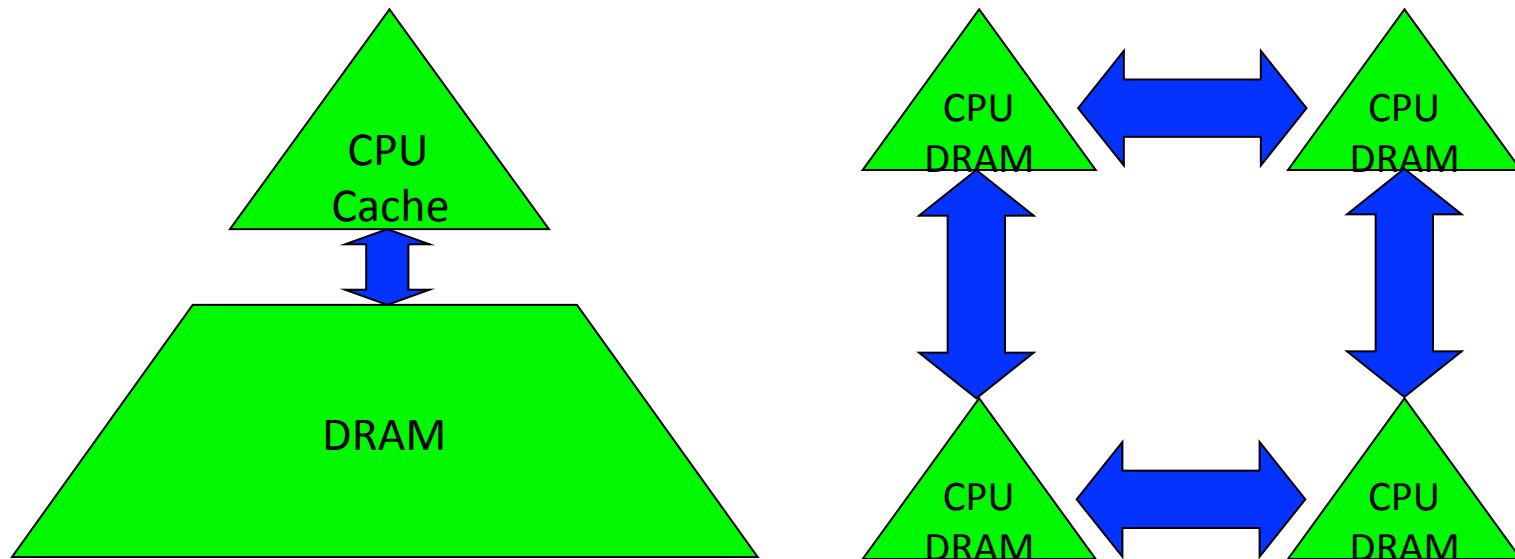
EECS & Math Departments

UC Berkeley

Why avoid communication? (1/3)

Algorithms have two costs (measured in time or energy):

1. Arithmetic (FLOPS)
2. Communication: moving data between
 - levels of a memory hierarchy (sequential case)
 - processors over a network (parallel case).



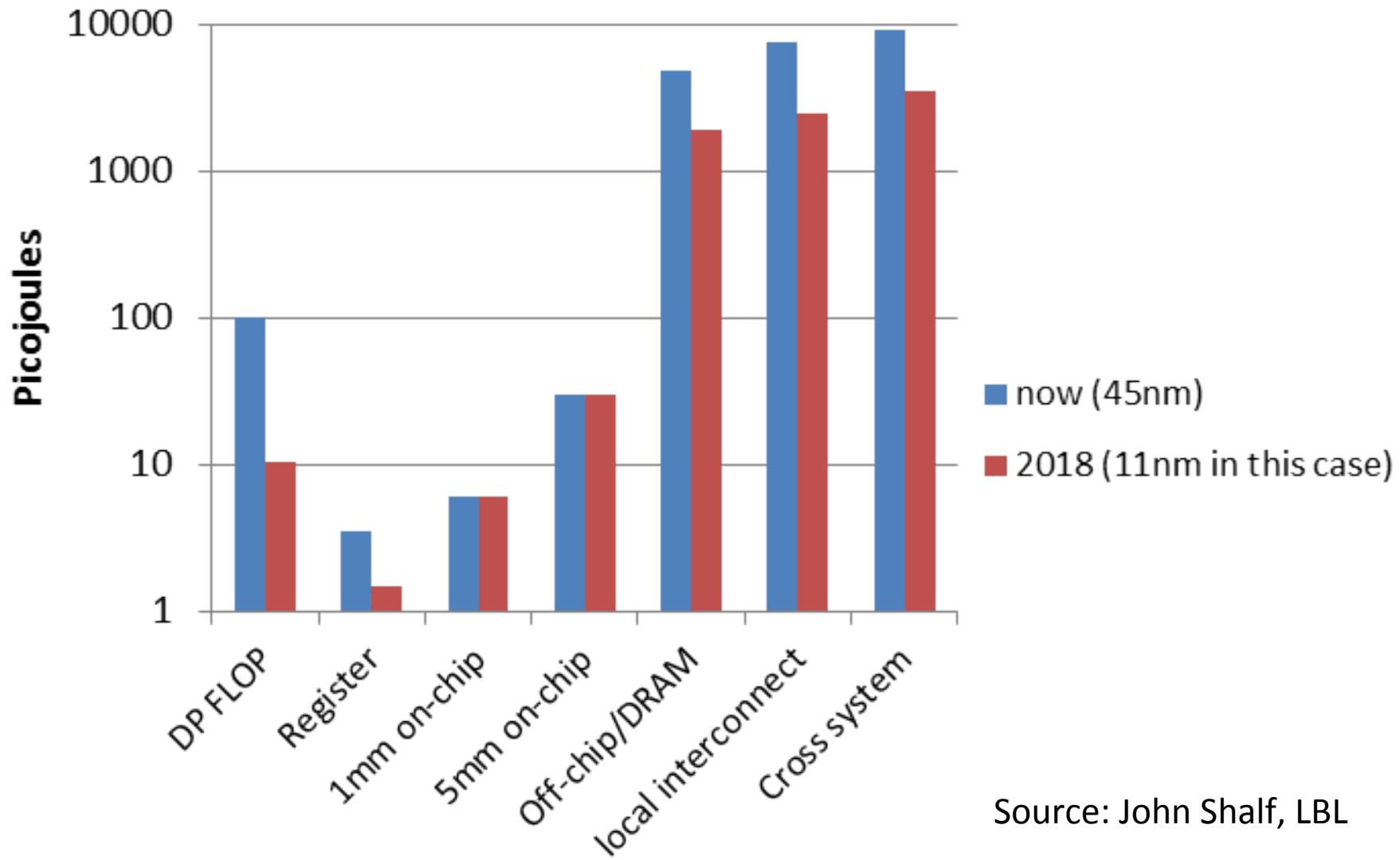
Why avoid communication? (2/3)

- Running time of an algorithm is sum of 3 terms:
 - $\# \text{ flops} * \text{time_per_flop}$
 - $\# \text{ words moved} / \text{bandwidth}$
 - $\# \text{ messages} * \text{latency}$
- $\text{Time_per_flop} \ll 1/\text{bandwidth} \ll \text{latency}$
 - Gaps growing exponentially with time [FOSC]

Annual improvements			
Time_per_flop		Bandwidth	Latency
59%	Network	26%	15%
	DRAM	23%	5%

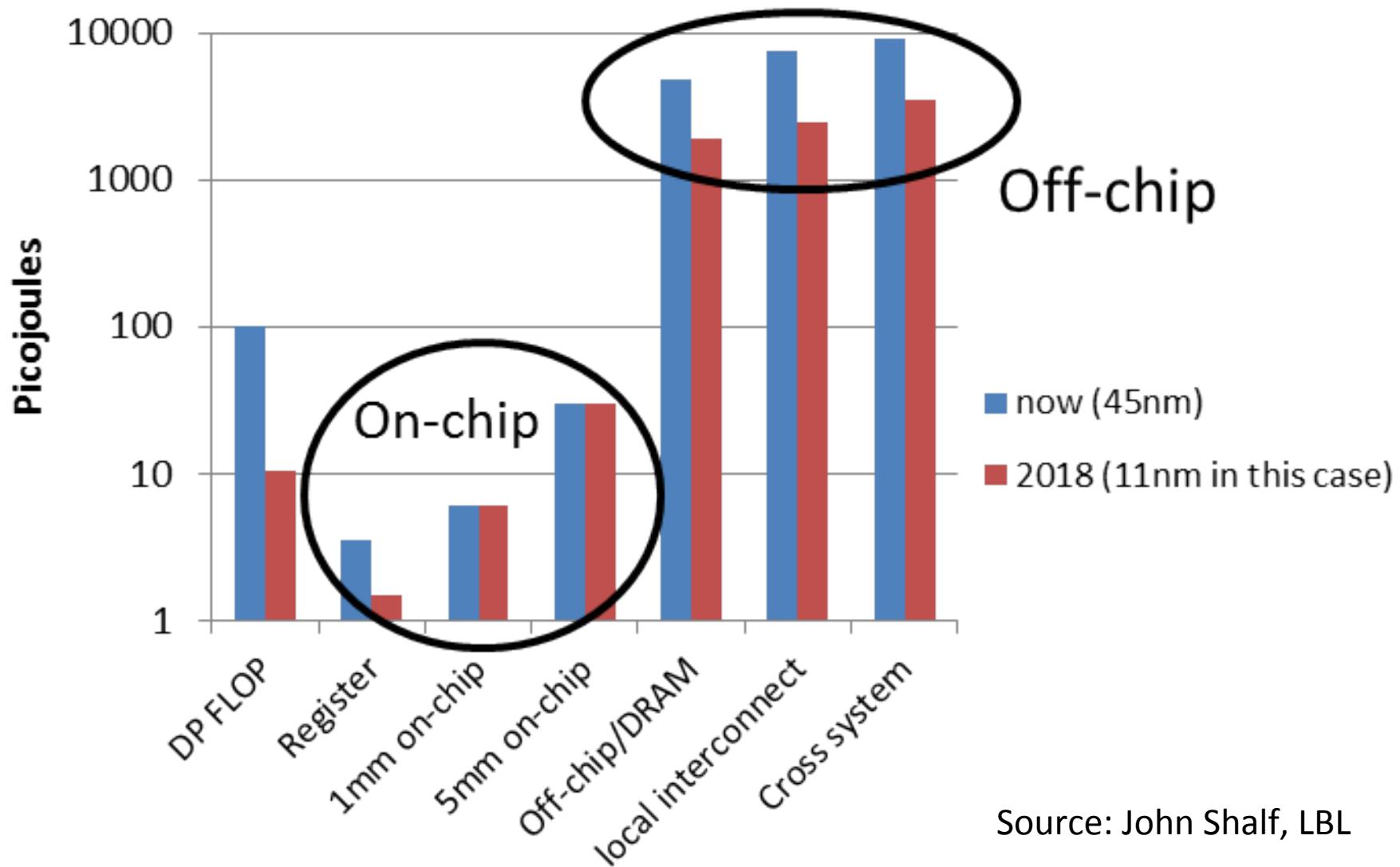
- Avoid communication to save time

Why Minimize Communication? (3/3)



Why Minimize Communication? (3/3)

Minimize communication to save energy



Source: John Shalf, LBL

Goals

- Redesign algorithms to *avoid* communication
 - Between all memory hierarchy levels
 - L1 \leftrightarrow L2 \leftrightarrow DRAM \leftrightarrow network, etc
- Attain lower bounds if possible
 - Current algorithms often far from lower bounds
 - Large speedups and energy savings possible

President Obama cites Communication-Avoiding Algorithms in the FY 2012 Department of Energy Budget Request to Congress:

“New Algorithm Improves Performance and Accuracy on Extreme-Scale Computing Systems. **On modern computer architectures, communication between processors takes longer than the performance of a floating point arithmetic operation by a given processor.** ASCR researchers have developed a new method, derived from commonly used linear algebra methods, to **minimize communications between processors and the memory hierarchy, by reformulating the communication patterns specified within the algorithm.** This method has been implemented in the TRILINOS framework, a highly-regarded suite of software, which provides functionality for researchers around the world to solve large scale, complex multi-physics problems.”

FY 2010 Congressional Budget, Volume 4, FY2010 Accomplishments, Advanced Scientific Computing Research (ASCR), pages 65-67.

CA-GMRES (Hoemmen, Mohiyuddin, Yelick, JD)
“Tall-Skinny” QR (Grigori, Hoemmen, Langou, JD)

Outline

- Survey state of the art of CA (Comm-Avoiding) algorithms
 - Review previous Matmul algorithms
 - CA $O(n^3)$ 2.5D Matmul
 - TSQR: Tall-Skinny QR
 - CA $O(n^3)$ 2.5D LU
 - CA Strassen Matmul
- Beyond linear algebra
 - Extending lower bounds to any algorithm with arrays
 - Communication-optimal N-body algorithm
- CA-Krylov methods

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Summary of CA Linear Algebra

- “Direct” Linear Algebra
 - Lower bounds on communication for linear algebra problems like $Ax=b$, least squares, $Ax = \lambda x$, SVD, etc
 - Mostly not attained by algorithms in standard libraries
 - New algorithms that attain these lower bounds
 - Being added to libraries: Sca/LAPACK, PLASMA, MAGMA
 - Large speed-ups possible
 - Autotuning to find optimal implementation
- Ditto for “Iterative” Linear Algebra

Lower bound for all “n³-like” linear algebra

- Let M = “fast” memory size (per processor)

$$\text{#words_moved (per processor)} = \Omega(\text{\#flops (per processor)} / M^{1/2})$$

- Parallel case: assume either load or memory balanced
- Holds for
 - Matmul

Lower bound for all “n³-like” linear algebra

- Let M = “fast” memory size (per processor)

$$\# \text{words_moved (per processor)} = \Omega(\# \text{flops (per processor)} / M^{1/2})$$

$$\# \text{messages_sent} \geq \# \text{words_moved} / \text{largest_message_size}$$

- Parallel case: assume either load or memory balanced
- Holds for
 - Matmul, BLAS, LU, QR, eig, SVD, tensor contractions, ...
 - Some whole programs (sequences of these operations, no matter how individual ops are interleaved, eg A^k)
 - Dense and sparse matrices (where #flops << n³)
 - Sequential and parallel algorithms
 - Some graph-theoretic algorithms (eg Floyd-Warshall)

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SIAM SIAG/Linear Algebra Prize, 2012
Ballard, D., Holtz, Schwartz

Can we attain these lower bounds?

- Do conventional dense algorithms as implemented in LAPACK and ScaLAPACK attain these bounds?
 - Often not
- If not, are there other algorithms that do?
 - Yes, for much of dense linear algebra
 - New algorithms, with new numerical properties, new ways to encode answers, new data structures
 - Not just loop transformations (need those too!)
- Only a few sparse algorithms so far
- Lots of work in progress

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Naïve Matrix Multiply

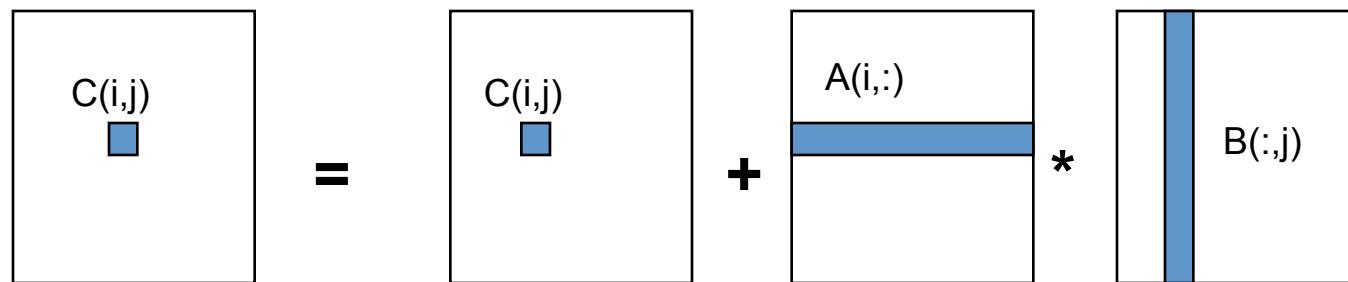
{implements $C = C + A * B$ }

for $i = 1$ to n

 for $j = 1$ to n

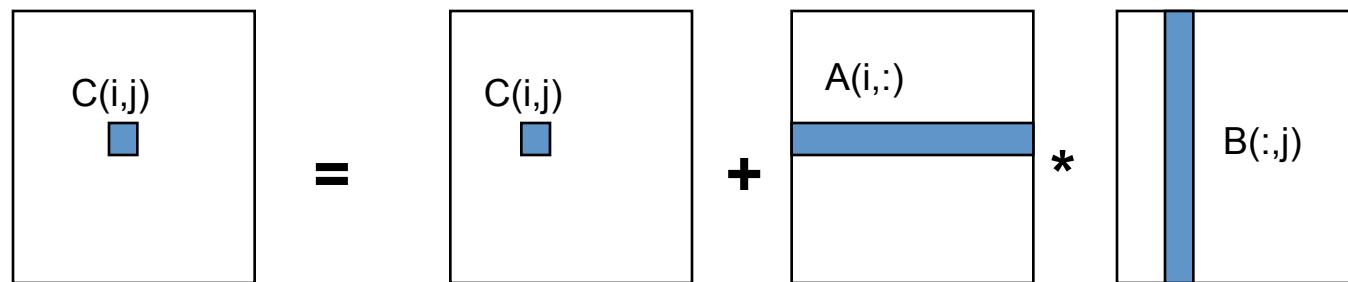
 for $k = 1$ to n

$$C(i,j) = C(i,j) + A(i,k) * B(k,j)$$



Naïve Matrix Multiply

```
{implements C = C + A*B}  
for i = 1 to n  
    {read row i of A into fast memory}  
    for j = 1 to n  
        {read C(i,j) into fast memory}  
        {read column j of B into fast memory}  
        for k = 1 to n  
            C(i,j) = C(i,j) + A(i,k) * B(k,j)  
        {write C(i,j) back to slow memory}
```



Naïve Matrix Multiply

{implements $C = C + A \cdot B$ }

for $i = 1$ to n

{read row i of A into fast memory} ... n^2 reads altogether

for $j = 1$ to n

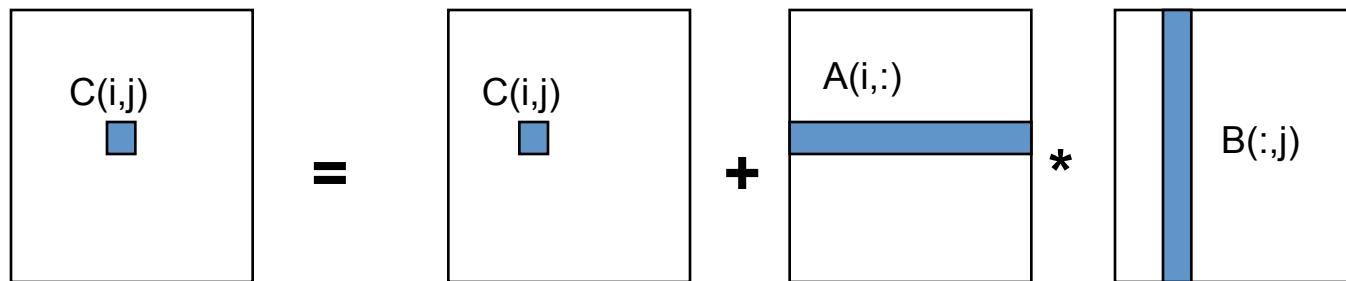
{read $C(i,j)$ into fast memory} ... n^2 reads altogether

{read column j of B into fast memory} ... n^3 reads altogether

for $k = 1$ to n

$$C(i,j) = C(i,j) + A(i,k) * B(k,j)$$

{write $C(i,j)$ back to slow memory} ... n^2 writes altogether

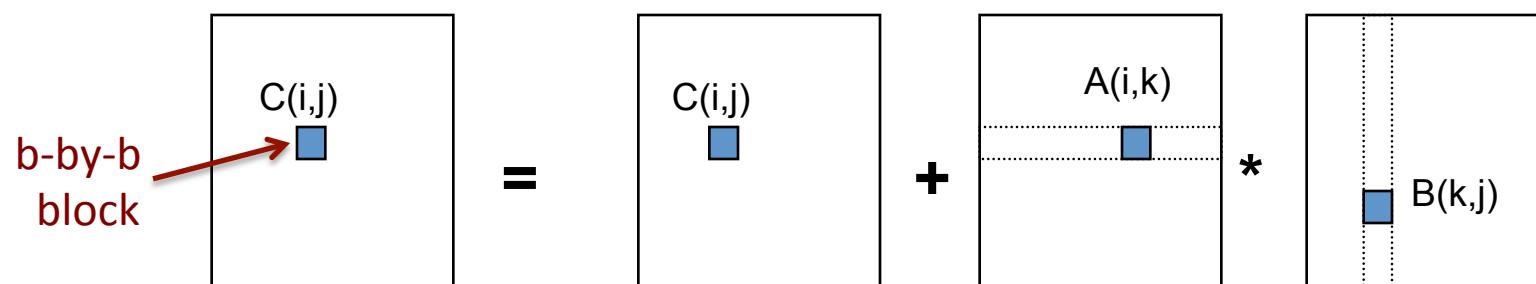


$n^3 + 3n^2$ reads/writes altogether – dominates $2n^3$ arithmetic

Blocked (Tiled) Matrix Multiply

Consider A, B, C to be n/b -by- n/b matrices of b -by- b subblocks where b is called the **block size**; assume 3 b -by- b blocks fit in fast memory

```
for i = 1 to n/b
    for j = 1 to n/b
        {read block C(i,j) into fast memory}
        for k = 1 to n/b
            {read block A(i,k) into fast memory}
            {read block B(k,j) into fast memory}
            C(i,j) = C(i,j) + A(i,k) * B(k,j) {do a matrix multiply on blocks}
            {write block C(i,j) back to slow memory}
```



Blocked (Tiled) Matrix Multiply

Consider A, B, C to be n/b -by- n/b matrices of b -by- b subblocks where b is called the **block size**; assume 3 b -by- b blocks fit in fast memory

for $i = 1$ to n/b

 for $j = 1$ to n/b

 {read block $C(i,j)$ into fast memory} ... $b^2 \times (n/b)^2 = n^2$ reads

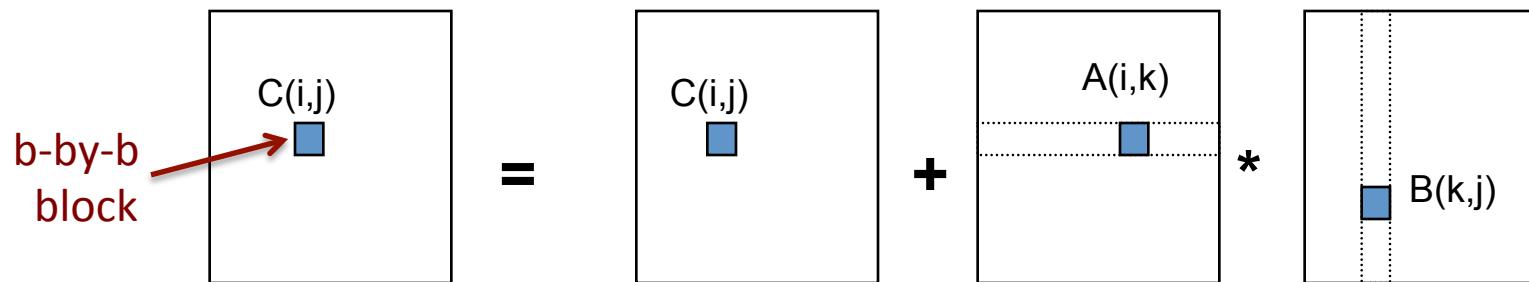
 for $k = 1$ to n/b

 {read block $A(i,k)$ into fast memory} ... $b^2 \times (n/b)^3 = n^3/b$ reads

 {read block $B(k,j)$ into fast memory} ... $b^2 \times (n/b)^3 = n^3/b$ reads

$C(i,j) = C(i,j) + A(i,k) * B(k,j)$ {do a matrix multiply on blocks}

 {write block $C(i,j)$ back to slow memory} ... $b^2 \times (n/b)^2 = n^2$ writes



$2n^3/b + 2n^2$ reads/writes $\ll 2n^3$ arithmetic - Faster!

Does blocked matmul attain lower bound?

- Recall: if 3 b-by-b blocks fit in fast memory of size M , then #reads/writes = $2n^3/b + 2n^2$
- Make b as large as possible: $3b^2 \leq M$, so #reads/writes $\geq 3^{1/2}n^3/M^{1/2} + 2n^2$
- Attains lower bound = $\Omega(\text{#flops} / M^{1/2})$
- But what if we don't know M ?
- Or if there are multiple levels of fast memory?
- How do we write the algorithm?

Recursive Matrix Multiplication (RMM) (1/2)

- For simplicity: square matrices with $n = 2^m$
- $C = \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} = A \cdot B = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \cdot \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}$
 $= \begin{pmatrix} A_{11} \cdot B_{11} + A_{12} \cdot B_{21} & A_{11} \cdot B_{12} + A_{12} \cdot B_{22} \\ A_{21} \cdot B_{11} + A_{22} \cdot B_{21} & A_{21} \cdot B_{12} + A_{22} \cdot B_{22} \end{pmatrix}$
- True when each A_{ij} etc 1×1 or $n/2 \times n/2$

```
func C = RMM (A, B, n)
    if n = 1, C = A * B, else
        { C11 = RMM (A11, B11, n/2) + RMM (A12, B21, n/2)
         C12 = RMM (A11, B12, n/2) + RMM (A12, B22, n/2)
         C21 = RMM (A21, B11, n/2) + RMM (A22, B21, n/2)
         C22 = RMM (A21, B12, n/2) + RMM (A22, B22, n/2) }
    return
```

Recursive Matrix Multiplication (RMM) (2/2)

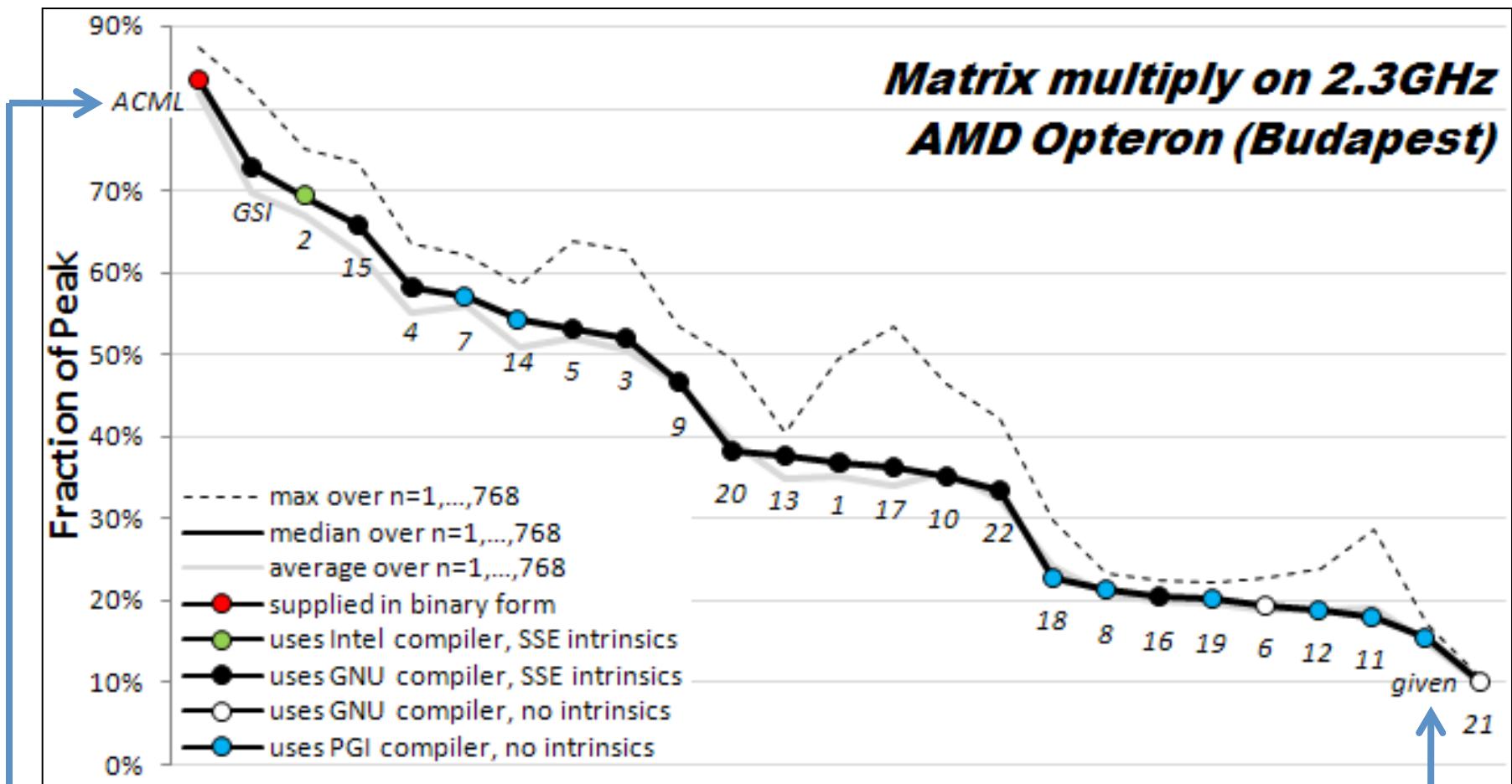
```
func C = RMM (A, B, n)
    if n=1, C = A * B, else
        { C11 = RMM (A11 , B11 , n/2) + RMM (A12 , B21 , n/2)
          C12 = RMM (A11 , B12 , n/2) + RMM (A12 , B22 , n/2)
          C21 = RMM (A21 , B11 , n/2) + RMM (A22 , B21 , n/2)
          C22 = RMM (A21 , B12 , n/2) + RMM (A22 , B22 , n/2) }
    return
```

$$\begin{aligned} A(n) &= \# \text{ arithmetic operations in } \text{RMM}(\dots, n) \\ &= 8 \cdot A(n/2) + 4(n/2)^2 \text{ if } n > 1, \text{ else } 1 \\ &= 2n^3 \dots \text{ same operations as usual, in different order} \end{aligned}$$

$$\begin{aligned} W(n) &= \# \text{ words moved between fast, slow memory by } \text{RMM}(\dots, n) \\ &= 8 \cdot W(n/2) + 12(n/2)^2 \text{ if } 3n^2 > M, \text{ else } 3n^2 \\ &= O(n^3 / M^{1/2} + n^2) \dots \text{ same as blocked matmul} \end{aligned}$$

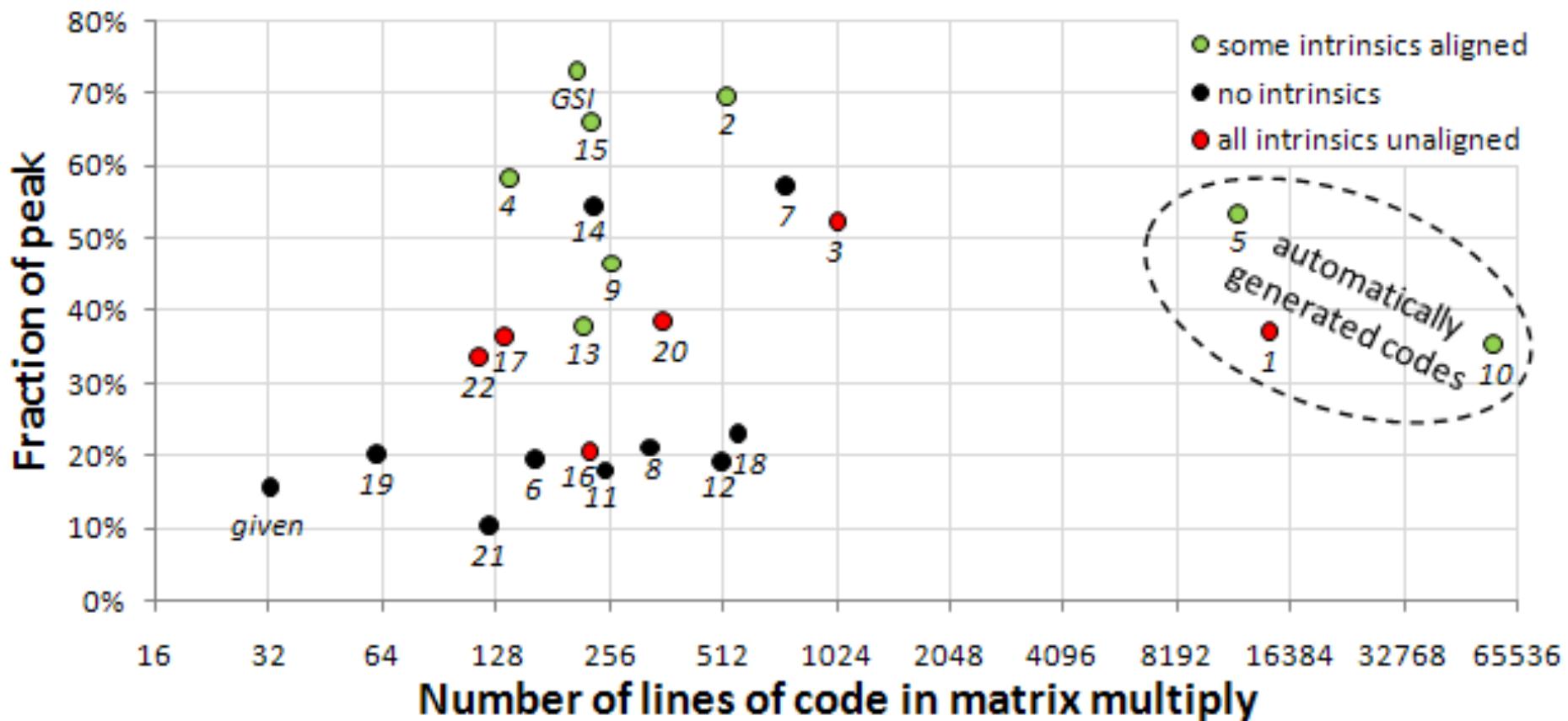
“Cache oblivious”, works for memory hierarchies, but not panacea

How hard is hand-tuning matmul, anyway?

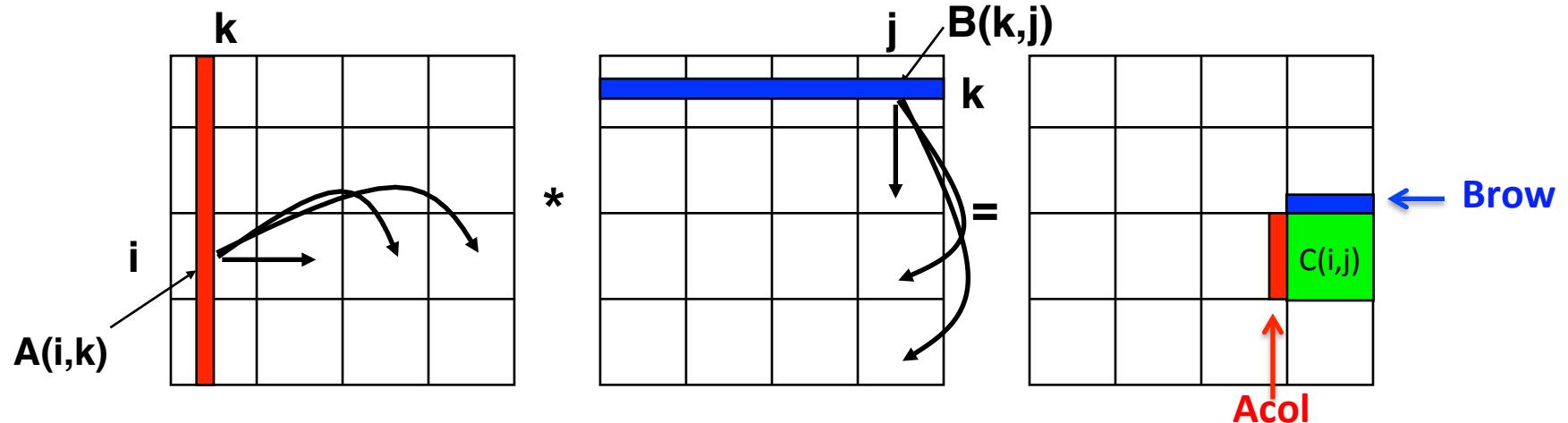


- Results of 22 student teams trying to tune matrix-multiply, in CS267 Spr09
- Students given “blocked” code to start with (7x faster than naïve)
 - Still hard to get close to vendor tuned performance (ACML) (another 6x)
- For more discussion, see www.cs.berkeley.edu/~volkov/cs267.sp09/hw1/results/

How hard is hand-tuning matmul, anyway?



SUMMA— $n \times n$ matmul on $P^{1/2} \times P^{1/2}$ grid (nearly) optimal using minimum memory $M=O(n^2/P)$



For $k=0$ to $n/b-1$... $b = \text{block size} = \#\text{cols in } A(i,k) = \#\text{rows in } B(k,j)$

for all $i = 1$ to $P^{1/2}$
 owner of **A(i,k)** broadcasts it to whole processor row (using binary tree)

for all $j = 1$ to $P^{1/2}$
 owner of **B(k,j)** broadcasts it to whole processor column (using bin. tree)

Receive A(i,k) into **Acol**

Receive B(k,j) into **Brow**

C_myproc = **C_myproc** + **Acol** * **Brow**

Summary of dense *parallel* algorithms attaining communication lower bounds

- Assume $n \times n$ matrices on P processors
- Minimum Memory per processor = $M = O(n^2 / P)$
- Recall lower bounds:
 $\#words_moved = \Omega((n^3 / P) / M^{1/2}) = \Omega(n^2 / P^{1/2})$
 $\#messages = \Omega((n^3 / P) / M^{3/2}) = \Omega(P^{1/2})$
- Does ScaLAPACK attain these bounds?
 - For $\#words_moved$: mostly, except nonsym. Eigenproblem
 - For $\#messages$: asymptotically worse, except Cholesky
- New algorithms attain all bounds, up to polylog(P) factors
 - Cholesky, LU, QR, Sym. and Nonsym eigenproblems, SVD

Can we do Better?

Can we do better?

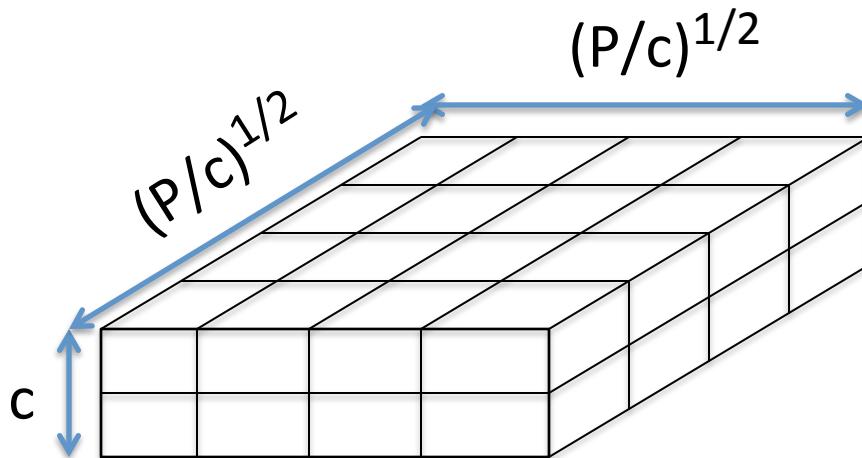
- Aren't we already optimal?
- Why assume $M = O(n^2/p)$, i.e. minimal?
 - Lower bound still true if more memory
 - Can we attain it?
- Special case: “3D Matmul”
 - Uses $M = O(n^2/p^{2/3})$
 - Dekel, Nassimi, Sahni [81], Bernsten [89], Agarwal, Chandra, Snir [90], Johnson [93], Agarwal, Balle, Gustavson, Joshi, Palkar [95]
 - Processors arranged in $p^{1/3} \times p^{1/3} \times p^{1/3}$ grid
 - Processor (i,j,k) performs $C(i,j) = C(i,j) + A(i,k)*B(k,j)$, where each submatrix is $n/p^{1/3} \times n/p^{1/3}$
- Not always that much memory available...

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2.5D Matrix Multiplication

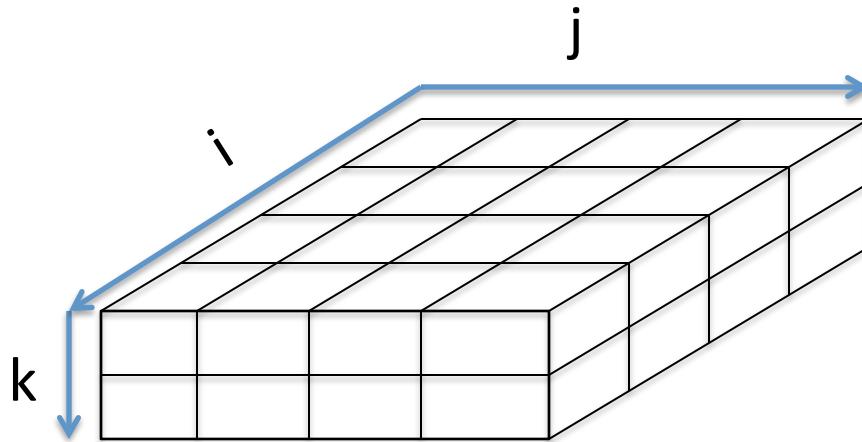
- Assume can fit cn^2/P data per processor, $c > 1$
- Processors form $(P/c)^{1/2} \times (P/c)^{1/2} \times c$ grid



Example: $P = 32, c = 2$

2.5D Matrix Multiplication

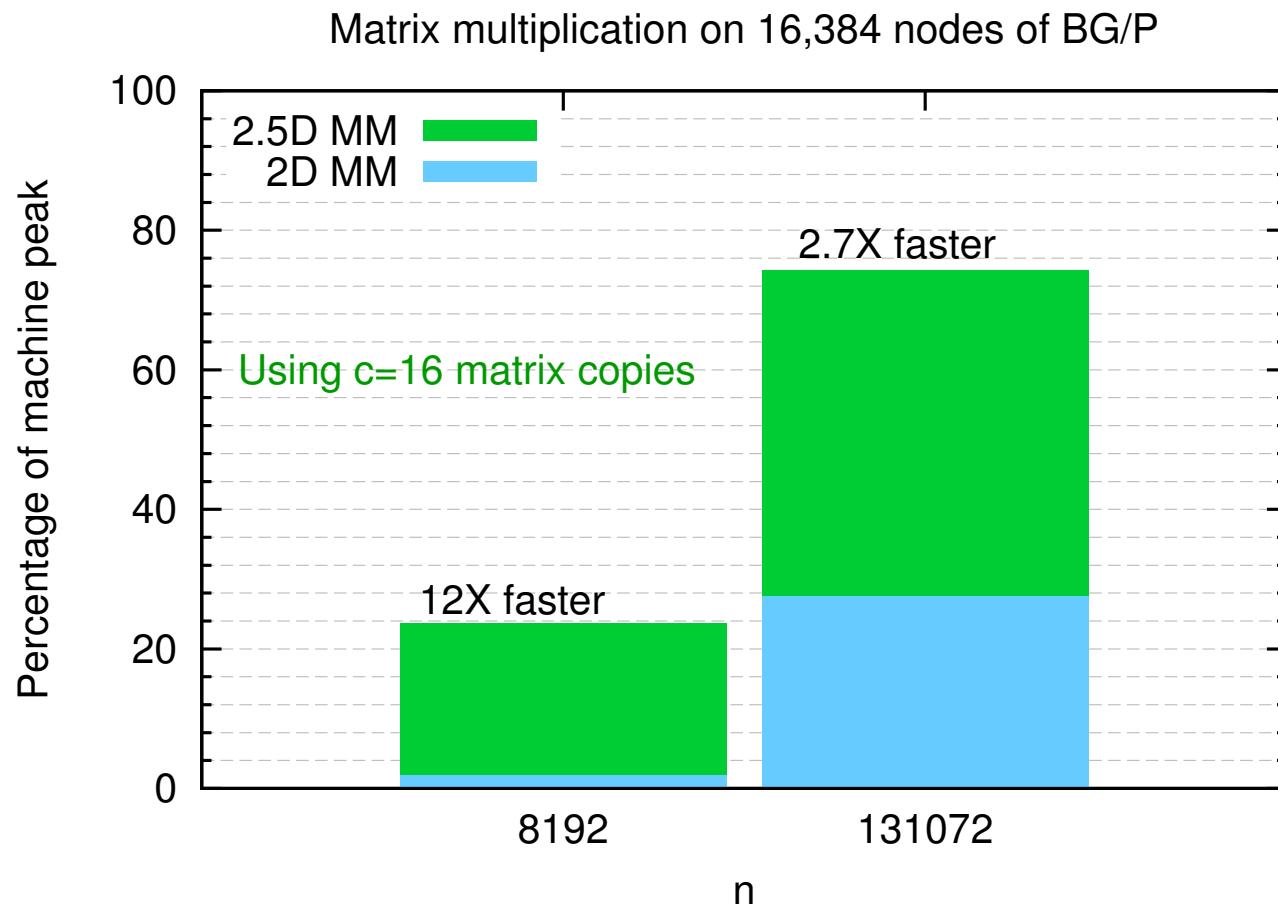
- Assume can fit cn^2/P data per processor, $c > 1$
- Processors form $(P/c)^{1/2} \times (P/c)^{1/2} \times c$ grid



Initially $P(i,j,0)$ owns $A(i,j)$ and $B(i,j)$ each of size $n(c/P)^{1/2} \times n(c/P)^{1/2}$

- (1) $P(i,j,0)$ broadcasts $A(i,j)$ and $B(i,j)$ to $P(i,j,k)$
- (2) Processors at level k perform $1/c$ -th of SUMMA, i.e. $1/c$ -th of $\sum_m A(i,m)*B(m,j)$
- (3) Sum-reduce partial sums $\sum_m A(i,m)*B(m,j)$ along k -axis so $P(i,j,0)$ owns $C(i,j)$

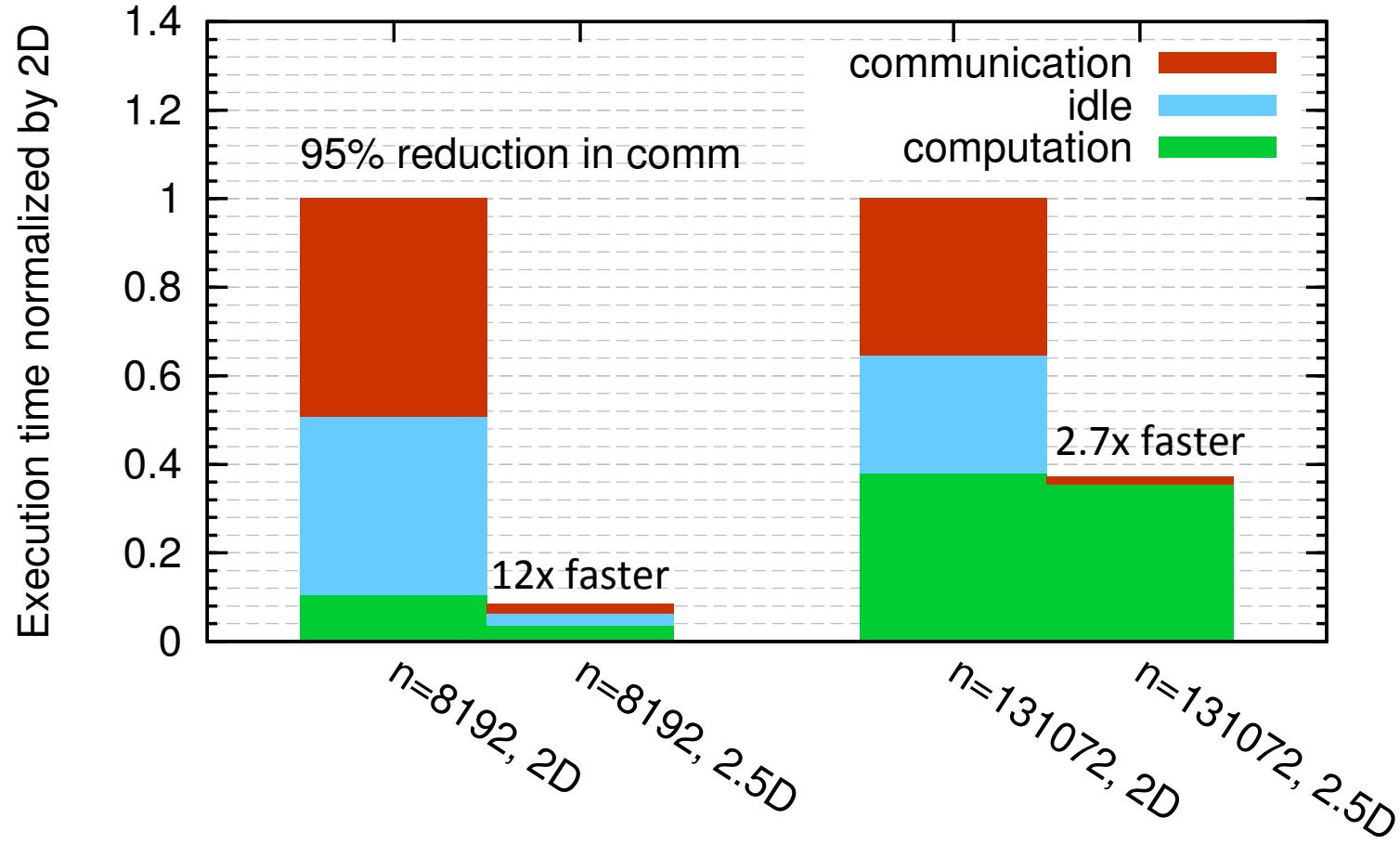
2.5D Matmul on BG/P, 16K nodes / 64K cores



2.5D Matmul on BG/P, 16K nodes / 64K cores

$c = 16$ copies

Matrix multiplication on 16,384 nodes of BG/P



Distinguished Paper Award, EuroPar'11 (Solomonik, D.)
SC'11 paper by Solomonik, Bhatele, D.

Perfect Strong Scaling – in Time and Energy (1/2)

- Every time you add a processor, you should use its memory M too
- Start with minimal number of procs: $PM = 3n^2$
- Increase P by a factor of c \rightarrow total memory increases by a factor of c
- Notation for timing model:
 - $\gamma_T, \beta_T, \alpha_T$ = secs per flop, per word_moved, per message of size m
- $T(cP) = n^3/(cP) [\gamma_T + \beta_T/M^{1/2} + \alpha_T/(mM^{1/2})]$
 $= T(P)/c$
- Notation for energy model:
 - $\gamma_E, \beta_E, \alpha_E$ = joules for same operations
 - δ_E = joules per word of memory used per sec
 - ε_E = joules per sec for leakage, etc.
- $E(cP) = cP \{ n^3/(cP) [\gamma_E + \beta_E/M^{1/2} + \alpha_E/(mM^{1/2})] + \delta_E MT(cP) + \varepsilon_E T(cP) \}$
 $= E(P)$

Perfect Strong Scaling – in Time and Energy (2/2)

- $T(cP) = n^3/(cP) [\gamma_T + \beta_T/M^{1/2} + \alpha_T/(mM^{1/2})] = T(P)/c$
- $E(cP) = cP \{ n^3/(cP) [\gamma_E + \beta_E/M^{1/2} + \alpha_E/(mM^{1/2})] + \delta_E MT(cP) + \varepsilon_E T(cP) \} = E(P)$
- Perfect scaling extends to N-body, Strassen, ...
- We can use these models to answer many questions, including:
- What is the minimum energy required for a computation?
- Given a maximum allowed runtime T , what is the minimum energy E needed to achieve it?
- Given a maximum energy budget E , what is the minimum runtime T that we can attain?
- The ratio $P = E/T$ gives us the average power required to run the algorithm. Can we minimize the average power consumed?
- Given an algorithm, problem size, number of processors and target energy efficiency (GFLOPS/W), can we determine a set of architectural parameters to describe a conforming computer architecture?

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TSQR: QR of a Tall, Skinny matrix

$$W = \begin{pmatrix} W_0 \\ \hline W_1 \\ \hline W_2 \\ \hline W_3 \end{pmatrix}$$

$$\begin{pmatrix} R_{00} \\ \hline R_{10} \\ \hline R_{20} \\ \hline R_{30} \end{pmatrix} = \begin{pmatrix} Q_{01} & R_{01} \\ \hline Q_{11} & R_{11} \end{pmatrix}$$

$$\begin{pmatrix} R_{01} \\ \hline R_{11} \end{pmatrix} = \begin{pmatrix} Q_{02} & R_{02} \end{pmatrix}$$

TSQR: QR of a Tall, Skinny matrix

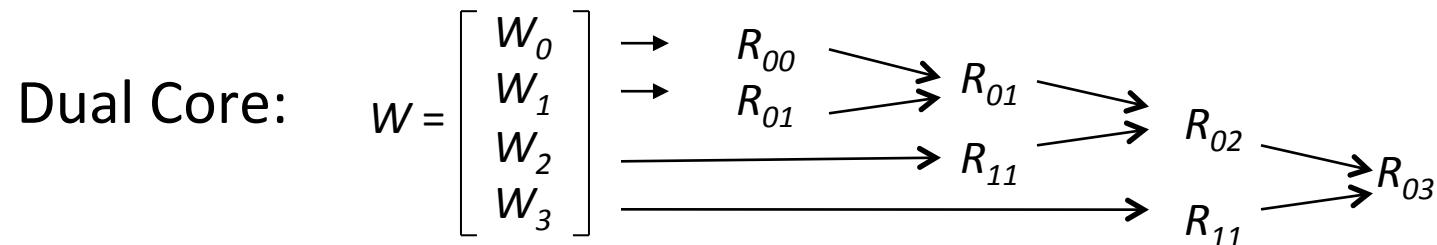
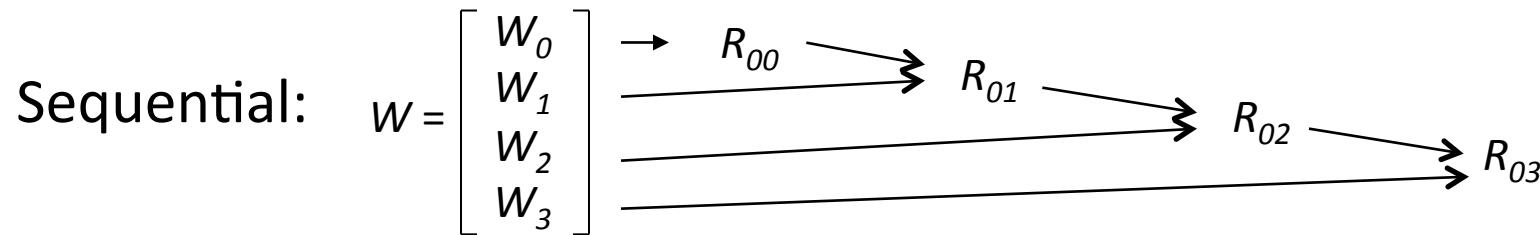
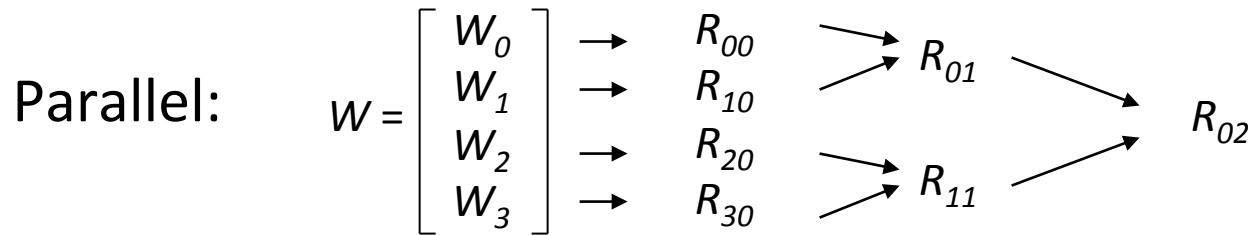
$$W = \begin{pmatrix} W_0 \\ W_1 \\ W_2 \\ W_3 \end{pmatrix} = \begin{pmatrix} Q_{00} & R_{00} \\ \hline Q_{10} & R_{10} \\ \hline Q_{20} & R_{20} \\ \hline Q_{30} & R_{30} \end{pmatrix} = \begin{pmatrix} \color{red}{Q_{00}} \\ \color{red}{Q_{10}} \\ \color{red}{Q_{20}} \\ \color{red}{Q_{30}} \end{pmatrix} \cdot \begin{pmatrix} R_{00} \\ R_{10} \\ R_{20} \\ R_{30} \end{pmatrix}$$

$$\begin{pmatrix} R_{00} \\ R_{10} \\ \hline R_{20} \\ R_{30} \end{pmatrix} = \begin{pmatrix} Q_{01} & R_{01} \\ \hline Q_{11} & R_{11} \end{pmatrix} = \begin{pmatrix} \color{red}{Q_{01}} \\ \color{red}{Q_{11}} \end{pmatrix} \cdot \begin{pmatrix} R_{01} \\ R_{11} \end{pmatrix}$$

$$\begin{pmatrix} R_{01} \\ R_{11} \end{pmatrix} = \begin{pmatrix} \color{red}{Q_{02}} & \color{red}{R_{02}} \end{pmatrix}$$

$$\text{Output} = \{ Q_{00}, Q_{10}, Q_{20}, Q_{30}, Q_{01}, Q_{11}, Q_{02}, R_{02} \}$$

TSQR: An Architecture-Dependent Algorithm



Multicore / Multisocket / Multirack / Multisite / Out-of-core: ?

Can choose reduction tree dynamically

TSQR Performance Results

- Parallel
 - Intel Clovertown
 - Up to **8x** speedup (8 core, dual socket, 10M x 10)
 - Pentium III cluster, Dolphin Interconnect, MPICH
 - Up to **6.7x** speedup (16 procs, 100K x 200)
 - BlueGene/L
 - Up to **4x** speedup (32 procs, 1M x 50)
 - Tesla C 2050 / Fermi
 - Up to **13x** ($110,592 \times 100$)
 - Grid – **4x** on 4 cities vs 1 city (Dongarra, Langou et al)
 - Cloud – **1.6x slower than accessing data twice** (Gleich and Benson)
- Sequential
 - “**Infinite speedup**” for out-of-core on PowerPC laptop
 - As little as 2x slowdown vs (predicted) infinite DRAM
 - LAPACK with virtual memory never finished
- SVD costs about the same
- Joint work with Grigori, Hoemmen, Langou, Anderson, Ballard, Keutzer, others

Outline

- Survey state of the art of CA (Comm-Avoiding) algorithms
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Back to LU: Using similar idea for TSLU as TSQR: Use reduction tree, to do “Tournament Pivoting”

$$W^{n \times b} = \begin{pmatrix} W_1 \\ W_2 \\ W_3 \\ W_4 \end{pmatrix} = \begin{pmatrix} P_1 \cdot L_1 \cdot U_1 \\ P_2 \cdot L_2 \cdot U_2 \\ P_3 \cdot L_3 \cdot U_3 \\ P_4 \cdot L_4 \cdot U_4 \end{pmatrix}$$

Choose b pivot rows of W_1 , call them W'_1
 Choose b pivot rows of W_2 , call them W'_2
 Choose b pivot rows of W_3 , call them W'_3
 Choose b pivot rows of W_4 , call them W'_4

$$\begin{pmatrix} W'_1 \\ W'_2 \\ \hline W'_3 \\ W'_4 \end{pmatrix} = \begin{pmatrix} P_{12} \cdot L_{12} \cdot U_{12} \\ \hline P_{34} \cdot L_{34} \cdot U_{34} \end{pmatrix}$$

Choose b pivot rows, call them W'_{12} ,
 Choose b pivot rows, call them W'_{34}

$$\begin{pmatrix} W'_{12} \\ W'_{34} \end{pmatrix} = P_{1234} \cdot L_{1234} \cdot U_{1234}$$

Choose b pivot rows

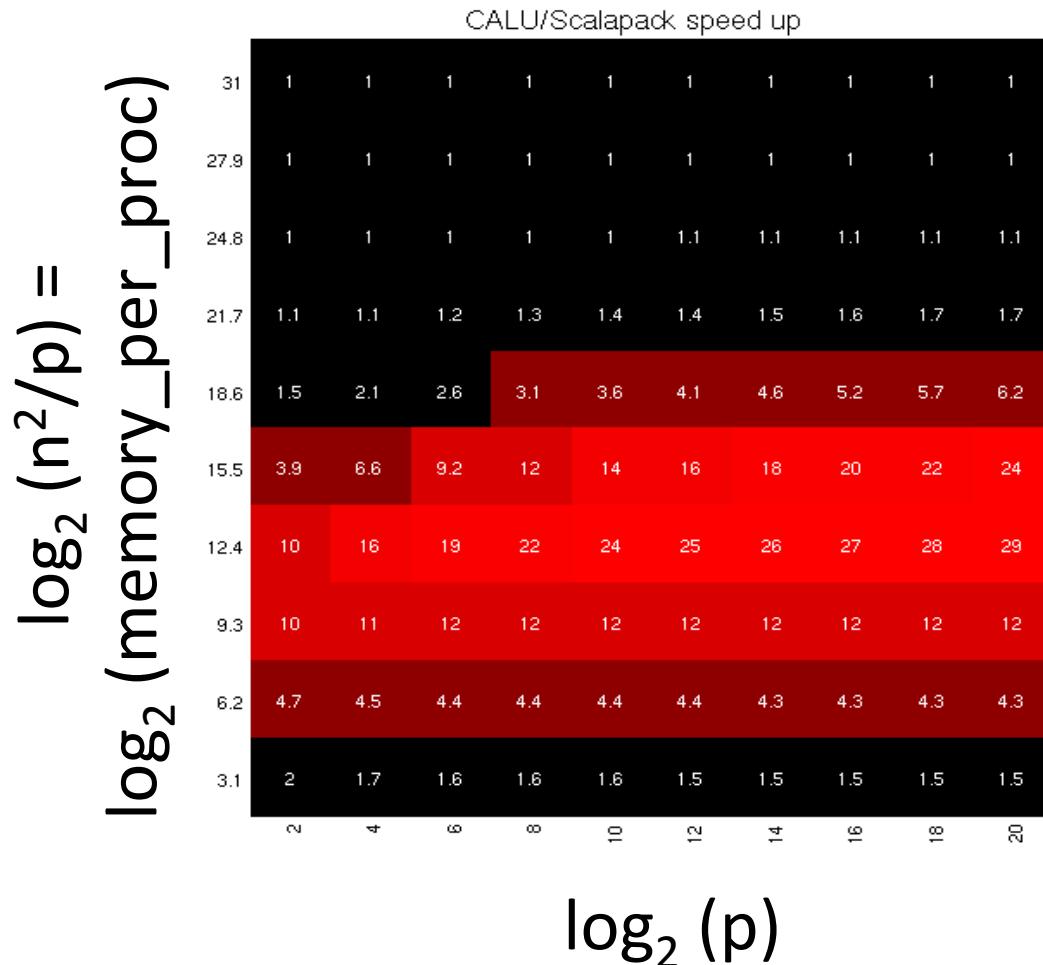
- Go back to W and use these b pivot rows
 - Move them to top, do LU without pivoting
 - Extra work, but lower order term
- Thm: As numerically stable as Partial Pivoting on a larger matrix

Exascale Machine Parameters

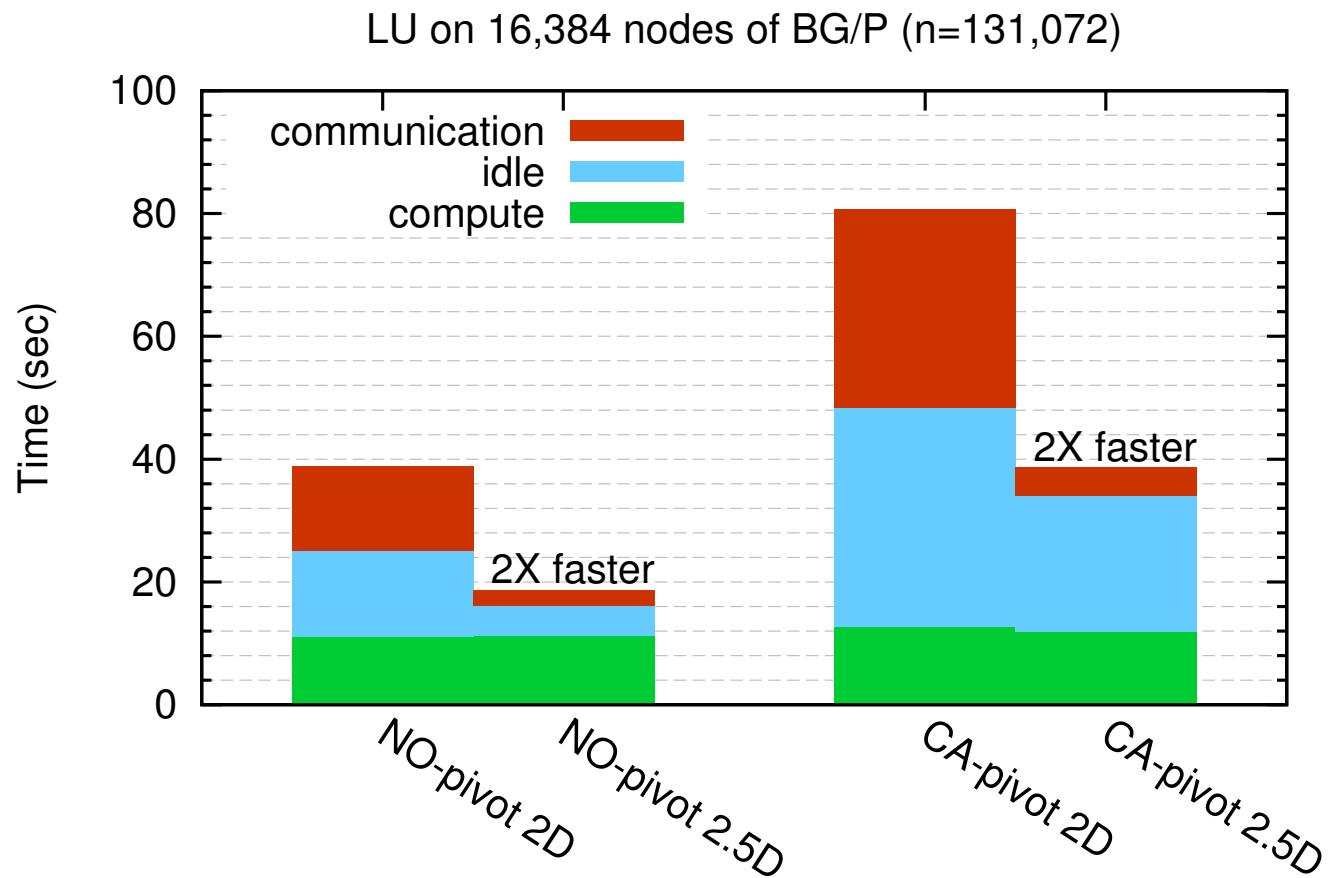
Source: DOE Exascale Workshop

- $2^{20} \approx 1,000,000$ nodes
- 1024 cores/node (a billion cores!)
- 100 GB/sec interconnect bandwidth
- 400 GB/sec DRAM bandwidth
- 1 microsec interconnect latency
- 50 nanosec memory latency
- 32 Petabytes of memory
- 1/2 GB total L1 on a node

Exascale predicted speedups for Gaussian Elimination: 2D CA-LU vs ScaLAPACK-LU



2.5D vs 2D LU With and Without Pivoting



Ongoing Work

- Lots more work on
 - Algorithms:
 - BLAS, LDL^T , QR with pivoting, other pivoting schemes, eigenproblems, ...
 - All-pairs-shortest-path, ...
 - Both 2D ($c=1$) and 2.5D ($c>1$)
 - But only bandwidth may decrease with $c>1$, not latency
 - Platforms:
 - Multicore, cluster, GPU, cloud, heterogeneous, low-energy, ...
 - Software:
 - Integration into Sca/LAPACK, PLASMA, MAGMA,...
- Integration into applications (on IBM BG/Q)
 - CTF (with ANL): symmetric tensor contractions

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Communication Lower Bounds for Strassen-like matmul algorithms

Classical
 $O(n^3)$ matmul:

$$\#words_moved = \Omega(M(n/M^{1/2})^3/P)$$

Strassen's
 $O(n^{\lg 7})$ matmul:

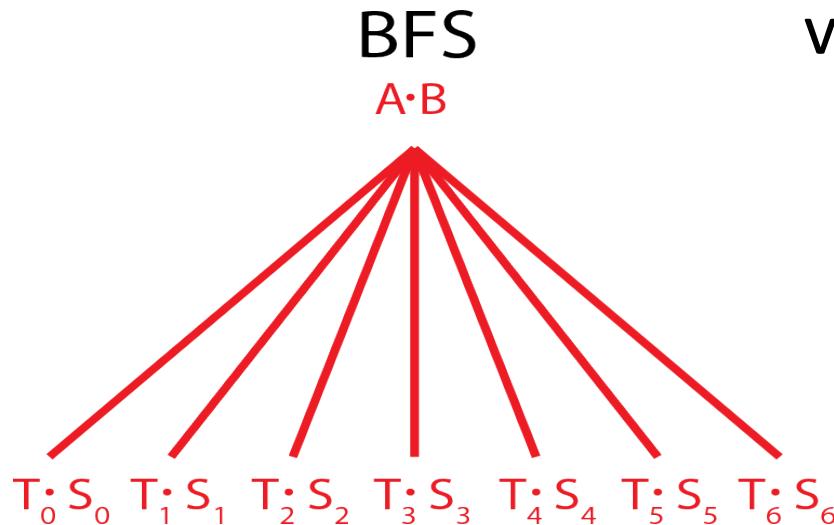
$$\#words_moved = \Omega(M(n/M^{1/2})^{\lg 7}/P)$$

Strassen-like
 $O(n^\omega)$ matmul:

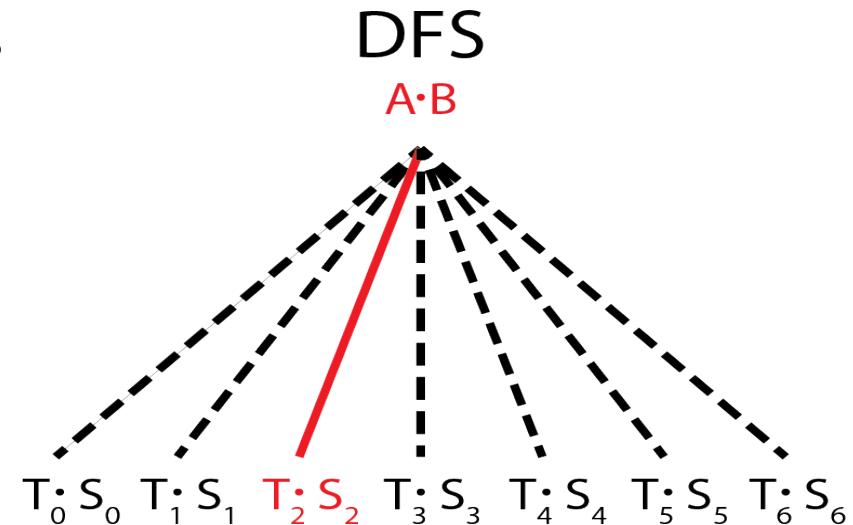
$$\#words_moved = \Omega(M(n/M^{1/2})^\omega/P)$$

- Proof: graph expansion (different from classical matmul)
 - Strassen-like: DAG must be “regular” and connected
- Extends up to $M = n^2 / p^{2/\omega}$
- Best Paper Prize (SPAA'11), Ballard, D., Holtz, Schwartz,
also in JACM
- Is the lower bound attainable?

Communication Avoiding Parallel Strassen (CAPS)



vs.



Runs all 7 multiplies in parallel
Each on P/7 processors
Needs 7/4 as much memory

Runs all 7 multiplies sequentially
Each on all P processors
Needs 1/4 as much memory

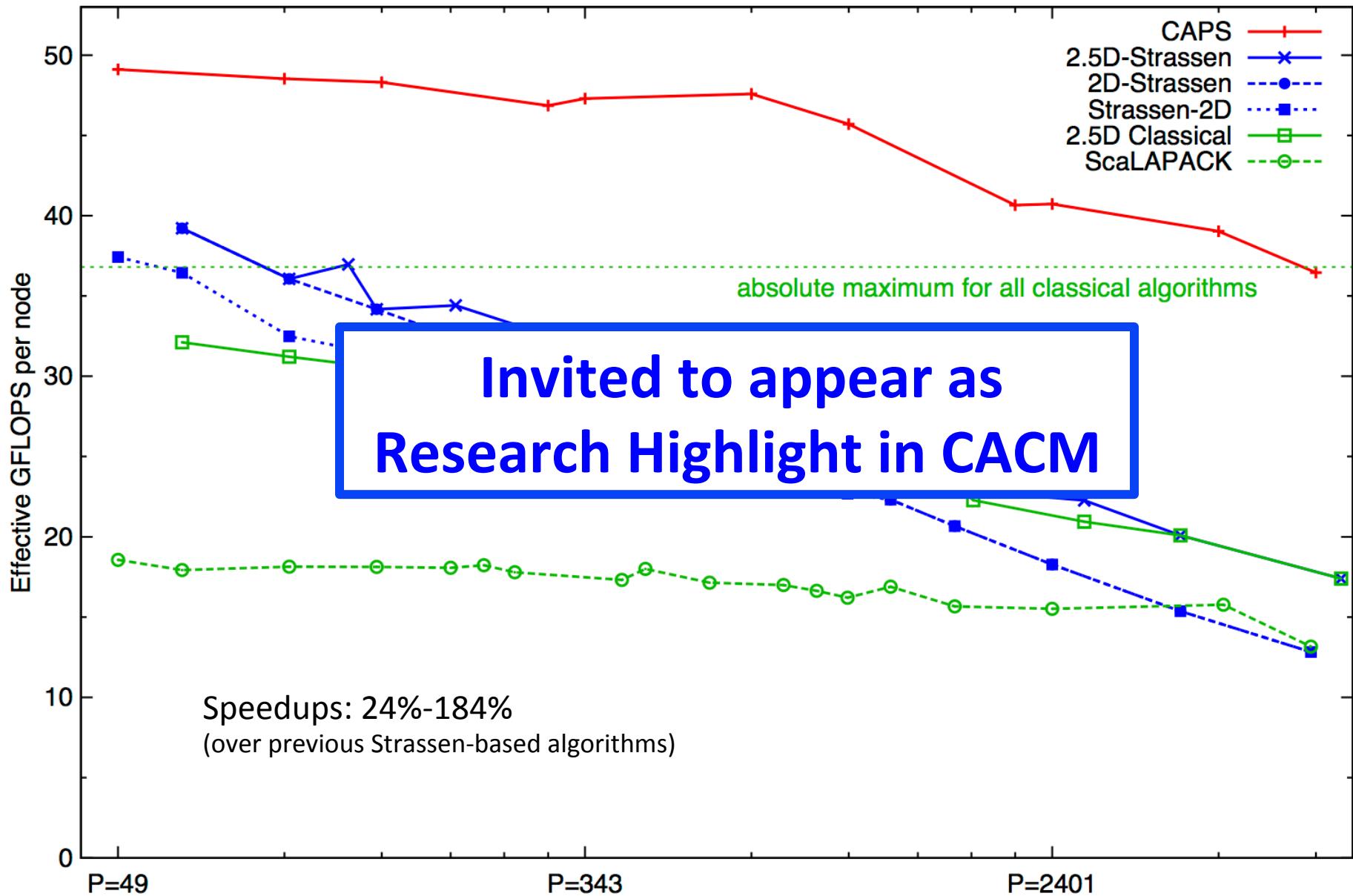
CAPS

If EnoughMemory and $P \geq 7$
then BFS step
else DFS step
end if

Best way to interleave
BFS and DFS is a
tuning parameter

Performance Benchmarking, Strong Scaling Plot

Franklin (Cray XT4) $n = 94080$



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Recall optimal sequential Matmul

- Naïve code
for $i=1:n$, for $j=1:n$, for $k=1:n$, $C(i,j) += A(i,k)*B(k,j)$
- “Blocked” code
for $i_1 = 1:b:n$, for $j_1 = 1:b:n$, for $k_1 = 1:b:n$
for $i_2 = 0:b-1$, for $j_2 = 0:b-1$, for $k_2 = 0:b-1$
 $i=i_1+i_2$, $j=j_1+j_2$, $k=k_1+k_2$
 $C(i,j) += A(i,k)*B(k,j)$ } $b \times b$ matmul
- Thm: Picking $b = M^{1/2}$ attains lower bound:
 $\#words_moved = \Omega(n^3/M^{1/2})$
- Where does $1/2$ come from?

New Thm applied to Matmul

- for $i=1:n$, for $j=1:n$, for $k=1:n$, $C(i,j) += A(i,k)*B(k,j)$
- Record array indices in matrix Δ

$$\Delta = \begin{pmatrix} i & j & k \\ 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 0 \end{pmatrix} \begin{matrix} A \\ B \\ C \end{matrix}$$

- Solve LP for $x = [x_i, x_j, x_k]^T$: $\max \mathbf{1}^T x$ s.t. $\Delta x \leq \mathbf{1}$
 - Result: $x = [1/2, 1/2, 1/2]^T$, $\mathbf{1}^T x = 3/2 = S_{HBL}$
- Thm: $\#words_moved = \Omega(n^3/M^{S_{HBL}-1}) = \Omega(n^3/M^{1/2})$
Attained by block sizes $M^{x_i}, M^{x_j}, M^{x_k} = M^{1/2}, M^{1/2}, M^{1/2}$

New Thm applied to Direct N-Body

- for $i=1:n$, for $j=1:n$, $F(i) += \text{force}(P(i), P(j))$
- Record array indices in matrix Δ

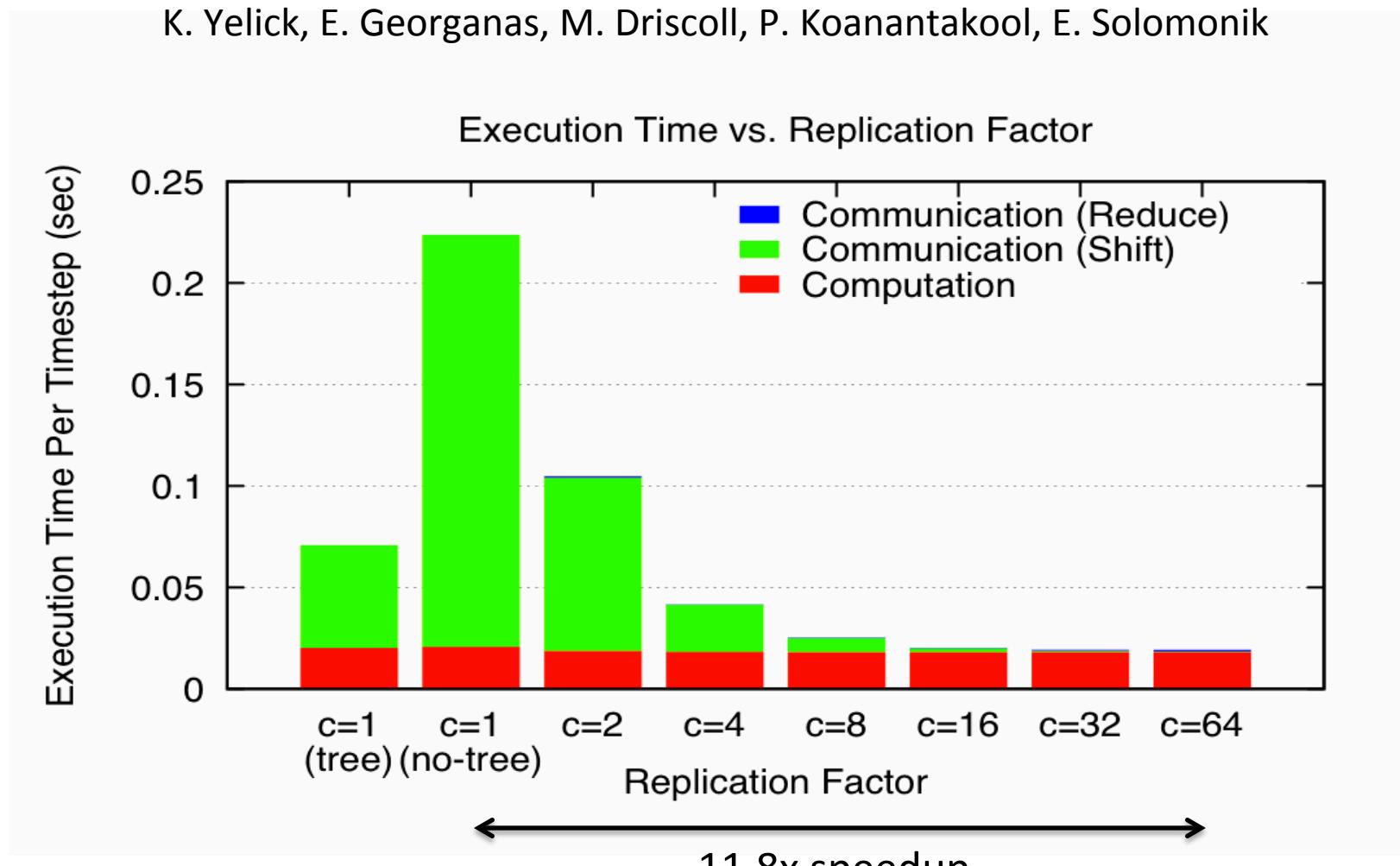
$$\Delta = \begin{pmatrix} & i & j \\ 1 & & 0 \\ 1 & & 0 \\ 0 & & 1 \end{pmatrix} \begin{matrix} F \\ P(i) \\ P(j) \end{matrix}$$

- Solve LP for $x = [x_i, x_j]^T$: $\max \mathbf{1}^T x$ s.t. $\Delta x \leq \mathbf{1}$
 - Result: $x = [1, 1]$, $\mathbf{1}^T x = 2 = S_{HBL}$
- Thm: $\#words_moved = \Omega(n^2/M^{S_{HBL}-1}) = \Omega(n^2/M^1)$
Attained by block sizes $M^{x_i}, M^{x_j} = M^1, M^1$

N-Body Speedups on IBM-BG/P (Intrepid)

8K cores, 32K particles

K. Yelick, E. Georganas, M. Driscoll, P. Koanantakool, E. Solomonik



New Thm applied to Random Code

- for $i_1=1:n$, for $i_2=1:n$, ... , for $i_6=1:n$

$$A_1(i_1, i_3, i_6) += \text{func1}(A_2(i_1, i_2, i_4), A_3(i_2, i_3, i_5), A_4(i_3, i_4, i_6))$$

$$A_5(i_2, i_6) += \text{func2}(A_6(i_1, i_4, i_5), A_3(i_3, i_4, i_6))$$

- Record array indices
in matrix Δ

	i_1	i_2	i_3	i_4	i_5	i_6	
A1	1	0	1	0	0	1	
A2	1	1	0	1	0	0	
A3	0	1	1	0	1	0	
A3,A4	0	0	1	1	0	1	
A5	0	0	1	1	0	1	
A6	1	0	0	1	1	0	

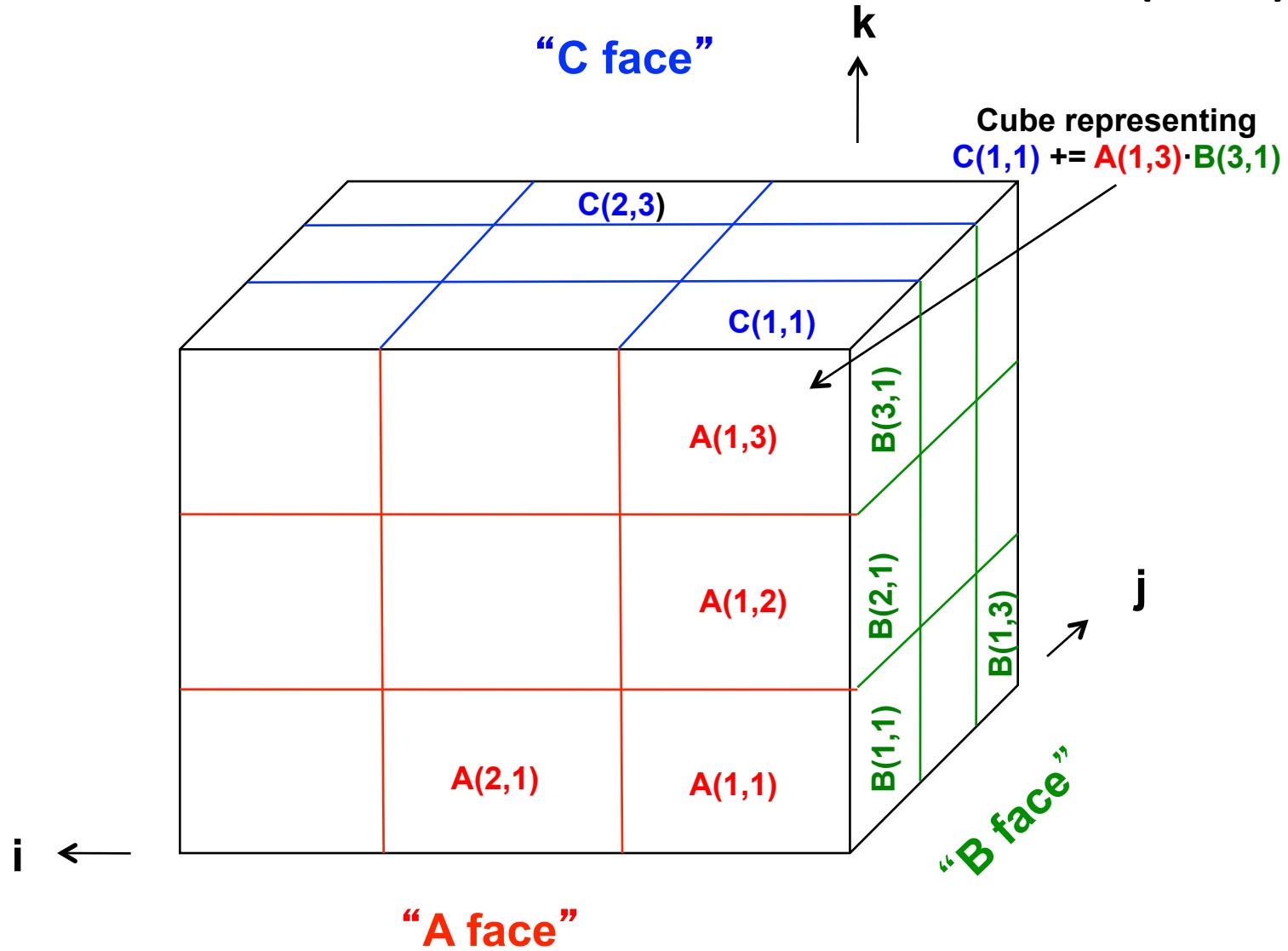
$\Delta =$

- Solve LP for $x = [x_1, \dots, x_7]^T$: $\max \mathbf{1}^T x$ s.t. $\Delta x \leq \mathbf{1}$
 - Result: $x = [2/7, 3/7, 1/7, 2/7, 3/7, 4/7]$, $\mathbf{1}^T x = 15/7 = S_{HBL}$
- Thm: $\#words_moved = \Omega(n^6/M^{S_{HBL}-1}) = \Omega(n^6/M^{8/7})$
Attained by block sizes $M^{2/7}, M^{3/7}, M^{1/7}, M^{2/7}, M^{3/7}, M^{4/7}$

Where do lower and matching upper bounds on communication come from? (1/3)

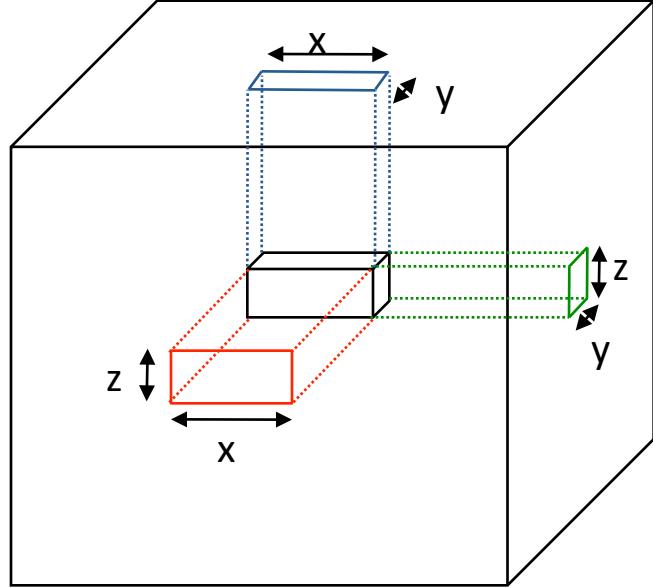
- Originally for $C = A * B$ by Irony/Tiskin/Toledo (2004)
- Proof idea
 - Suppose we can bound $\#\text{useful_operations} \leq G$ doable with data in fast memory of size M
 - So to do $F = \#\text{total_operations}$, need to fill fast memory F/G times, and so $\#\text{words_moved} \geq MF/G$
- Hard part: finding G
- Attaining lower bound
 - Need to “block” all operations to perform $\sim G$ operations on every chunk of M words of data

Proof of communication lower bound (2/3)

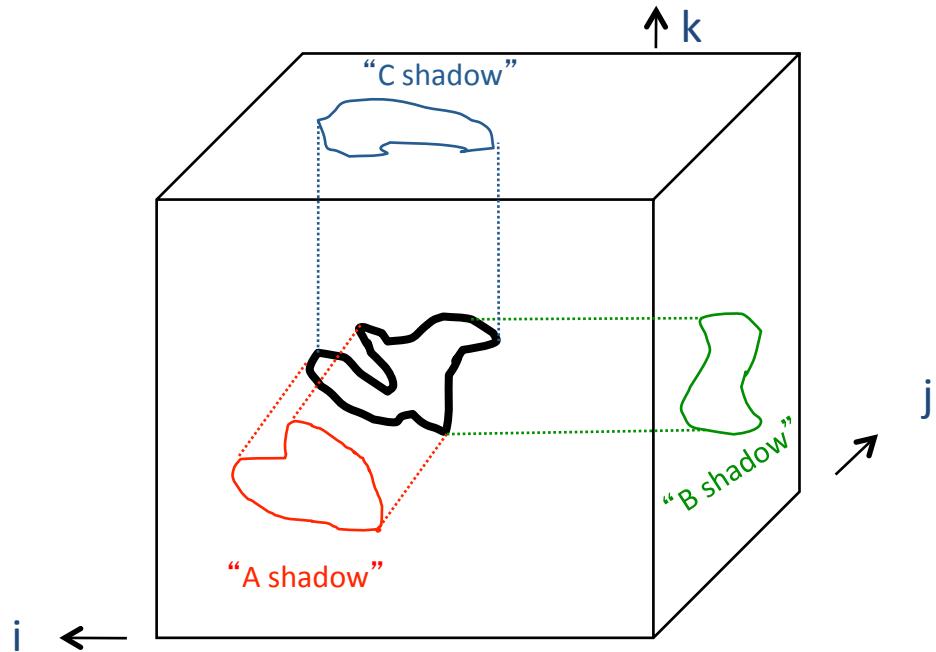


- If we have at most M “A squares”, M “B squares”, and M “C squares”, how many cubes G can we have? 58

Proof of communication lower bound (3/3)



$$\begin{aligned}
 G &= \# \text{ cubes in black box with side lengths } x, y \text{ and } z \\
 &= \text{Volume of black box} \\
 &= x \cdot y \cdot z \\
 &= (xz \cdot zy \cdot yx)^{1/2} \\
 &= (\#A\square s \cdot \#B\square s \cdot \#C\square s)^{1/2} \\
 &\leq M^{3/2}
 \end{aligned}$$



(i, k) is in “A shadow” if (i, j, k) in 3D set
 (j, k) is in “B shadow” if (i, j, k) in 3D set
 (i, j) is in “C shadow” if (i, j, k) in 3D set

Thm (Loomis & Whitney, 1949)

$$\begin{aligned}
 G &= \# \text{ cubes in 3D set} = \text{Volume of 3D set} \\
 &\leq (\text{area(A shadow)} \cdot \text{area(B shadow)} \cdot \text{area(C shadow)})^{1/2} \\
 &\leq M^{3/2}
 \end{aligned}$$

Approach to generalizing lower bounds

- Matmul

for $i=1:n$, for $j=1:n$, for $k=1:n$,

$$C(i,j) += A(i,k)*B(k,j)$$

=> for (i,j,k) in S = subset of Z^3

Access locations indexed by (i,j) , (i,k) , (k,j)

- General case

for $i_1=1:n$, for $i_2 = i_1:m$, ... for $i_k = i_3:i_4$

$$C(i_1+2*i_3-i_7) = \text{func}(A(i_2+3*i_4, i_1, i_2, i_1+i_2, \dots), B(\text{pnt}(3*i_4)), \dots)$$

$$D(\text{something else}) = \text{func}(\text{something else}), \dots$$

=> for (i_1, i_2, \dots, i_k) in S = subset of Z^k

Access locations indexed by group homomorphisms, eg

$$\phi_C(i_1, i_2, \dots, i_k) = (i_1+2*i_3-i_7)$$

$$\phi_A(i_1, i_2, \dots, i_k) = (i_2+3*i_4, i_1, i_2, i_1+i_2, \dots), \dots$$

- Can we bound #loop_iterations ($= |S|$)

given bounds on #points in its images, i.e. bounds on $|\phi_C(S)|$, $|\phi_A(S)|$, ... ?

General Communication Bound

- Given S subset of \mathbb{Z}^k , group homomorphisms ϕ_1, ϕ_2, \dots , bound $|S|$ in terms of $|\phi_1(S)|, |\phi_2(S)|, \dots, |\phi_m(S)|$
- Def: Hölder-Brascamp-Lieb LP (HBL-LP) for s_1, \dots, s_m :
for all subgroups $H < \mathbb{Z}^k$, $\text{rank}(H) \leq \sum_j s_j * \text{rank}(\phi_j(H))$
- Thm (Christ/Tao/Carbery/Bennett): Given s_1, \dots, s_m
$$|S| \leq \prod_j |\phi_j(S)|^{s_j}$$
- Thm: Given a program with array refs given by ϕ_j , choose s_j to minimize $s_{\text{HBL}} = \sum_j s_j$ subject to HBL-LP. Then
$$\#\text{words_moved} = \Omega (\#\text{iterations}/M^{s_{\text{HBL}}-1})$$

Is this bound attainable (1/2)?

- But first: Can we write it down?
- Thm: (bad news) HBL-LP reduces to Hilbert's 10th problem over Q (conjectured to be undecidable)
- Thm: (good news) Another LP with same solution is decidable (but expensive, so far)
- Thm: (better news) Easy to write down LP explicitly in many cases of interest (eg all $\phi_j = \{\text{subset of indices}\}$)
- Thm: (good news) Easy to approximate, i.e. get upper or lower bounds on s_{HBL}

Is this bound attainable (2/2)?

- Depends on loop dependencies
- Best case: none, or reductions (matmul)
- Thm: When all $\phi_j = \{\text{subset of indices}\}$, dual of HBL-LP gives optimal tile sizes:

$$\text{HBL-LP: } \text{minimize } \mathbf{1}^T * \mathbf{s} \text{ s.t. } \mathbf{s}^T * \Delta \geq \mathbf{1}^T$$

$$\text{Dual-HBL-LP: } \text{maximize } \mathbf{1}^T * \mathbf{x} \text{ s.t. } \Delta * \mathbf{x} \leq \mathbf{1}$$

Then for sequential algorithm, tile i_j by M^{x_j}

- Ex: Matmul: $\mathbf{s} = [1/2, 1/2, 1/2]^T = \mathbf{x}$
- Extends to unimodular transforms of indices

Ongoing Work

- Accelerate decision procedure for lower bounds
 - Ex: At most 3 arrays, or 4 loop nests
- Have yet to find a case where we cannot attain lower bound – can we prove this?
- Extend “perfect scaling” results for time and energy by using extra memory
 - “n.5D algorithms”
- Incorporate into compilers

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Avoiding Communication in Iterative Linear Algebra

- k-steps of iterative solver for sparse $Ax=b$ or $Ax=\lambda x$
 - Does k SpMVs with A and starting vector
 - Many such “Krylov Subspace Methods”
 - Conjugate Gradients (CG), GMRES, Lanczos, Arnoldi, ...
- Goal: minimize communication
 - Assume matrix “well-partitioned”
 - Serial implementation
 - Conventional: $O(k)$ moves of data from slow to fast memory
 - **New: $O(1)$ moves of data – optimal**
 - Parallel implementation on p processors
 - Conventional: $O(k \log p)$ messages (k SpMV calls, dot prods)
 - **New: $O(\log p)$ messages - optimal**
- Lots of speed up possible (modeled and measured)
 - Price: some redundant computation
 - Challenges: Poor partitioning, Preconditioning, Num. Stability

Communication Avoiding Kernels: The Matrix Powers Kernel : $[Ax, A^2x, \dots, A^kx]$

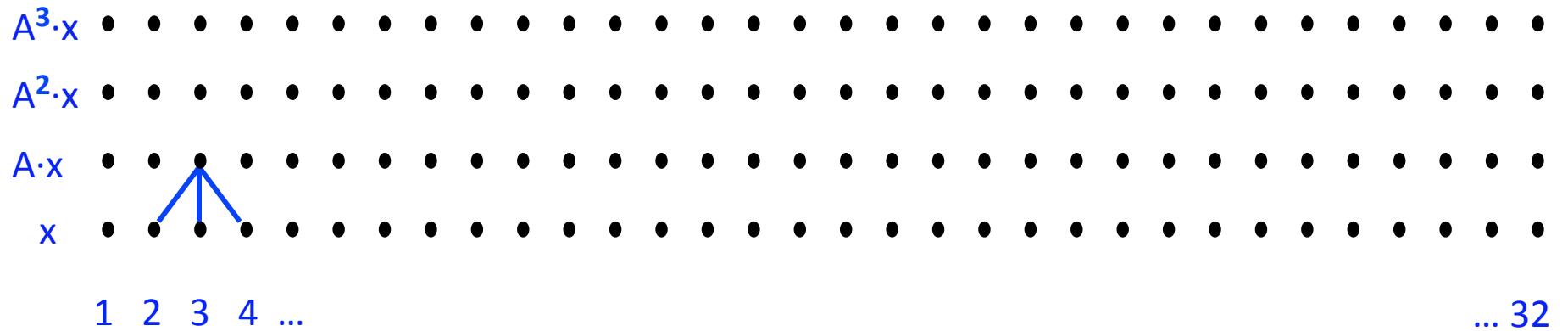
- Replace k iterations of $y = A \cdot x$ with $[Ax, A^2x, \dots, A^kx]$

- Example: A tridiagonal, $n=32$, $k=3$
 - Works for any “well-partitioned” A

Communication Avoiding Kernels:

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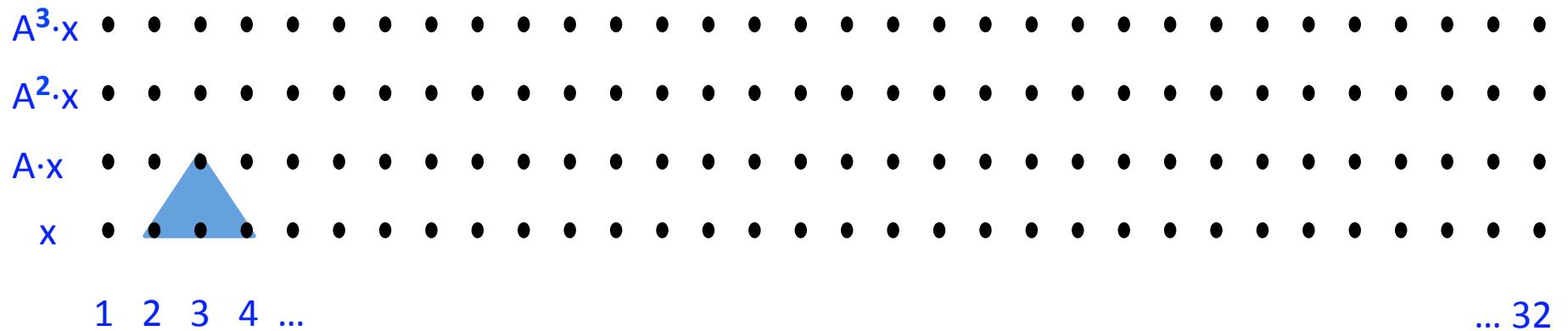


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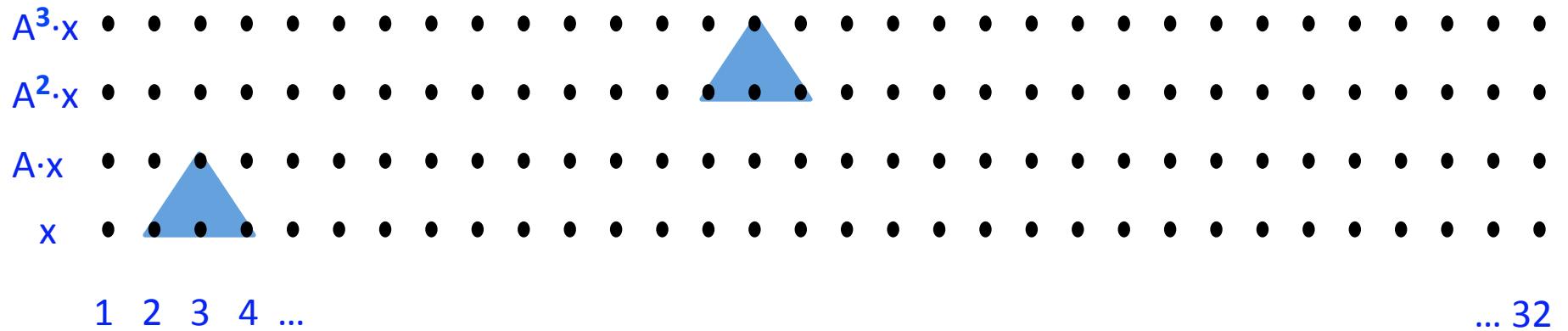


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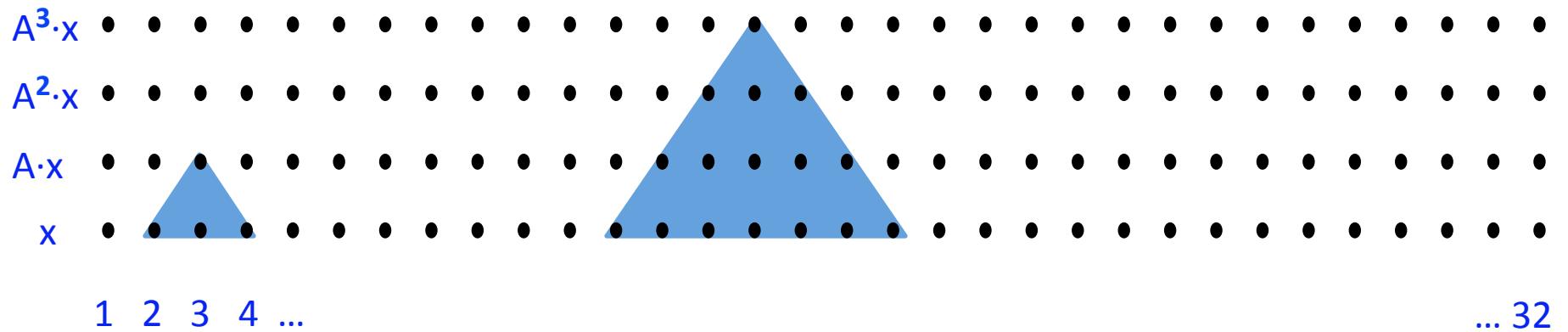


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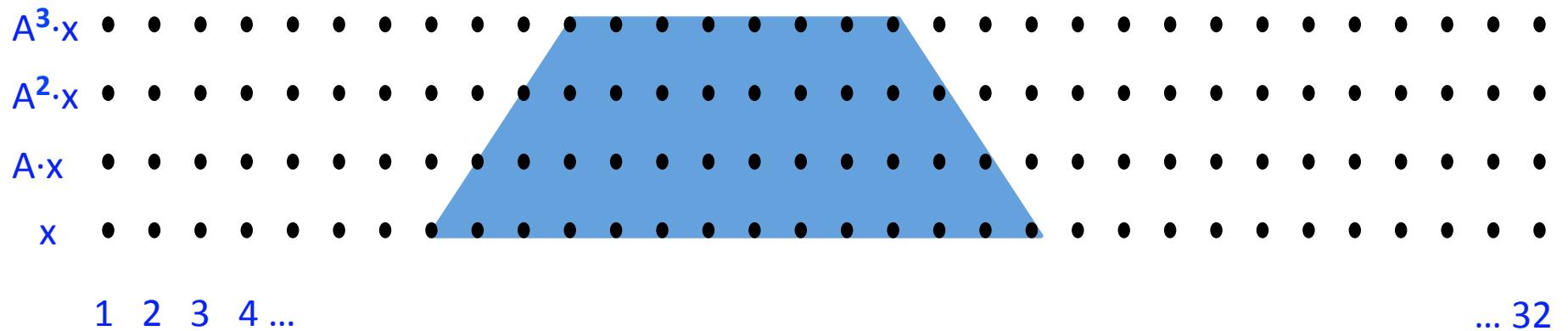


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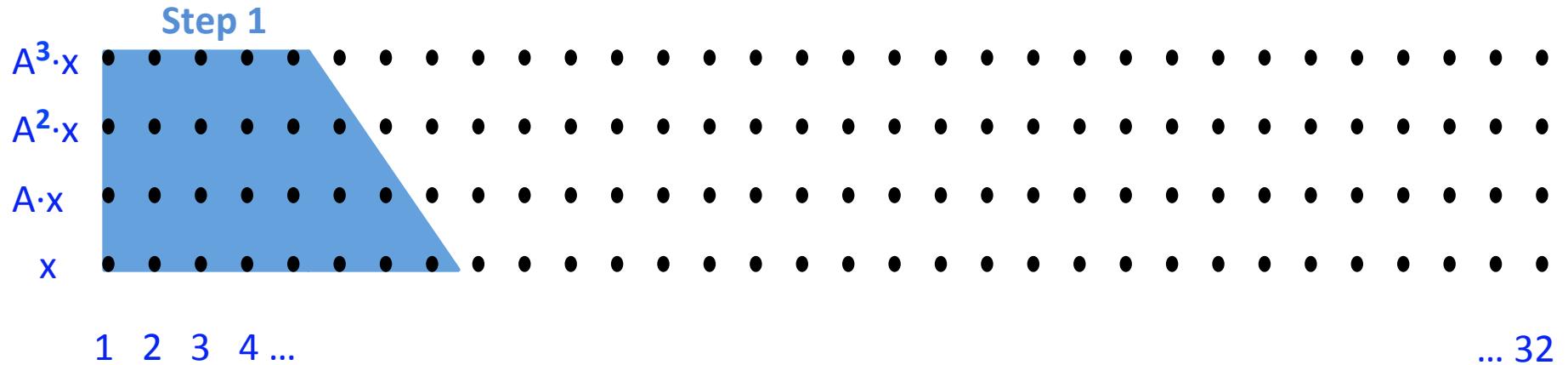


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- Sequential Algorithm

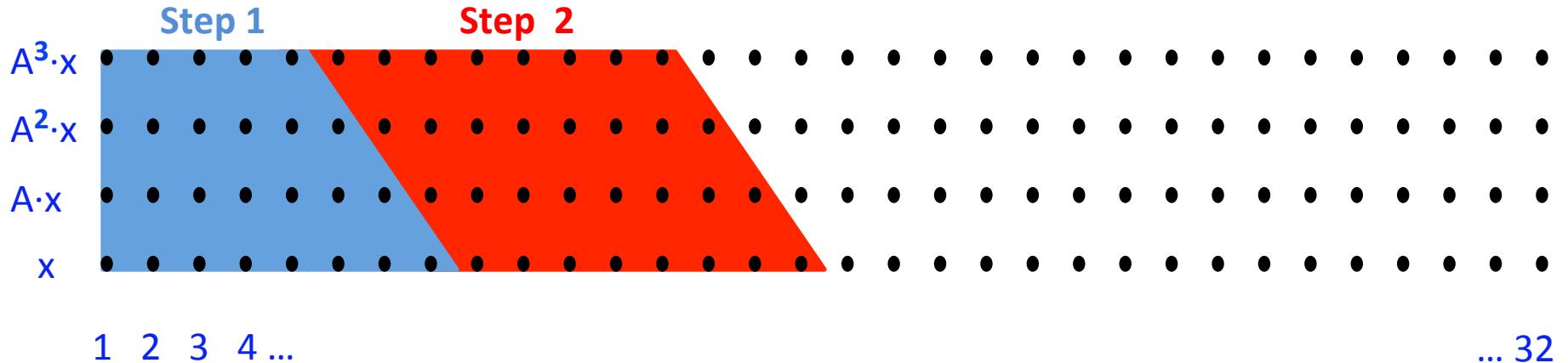


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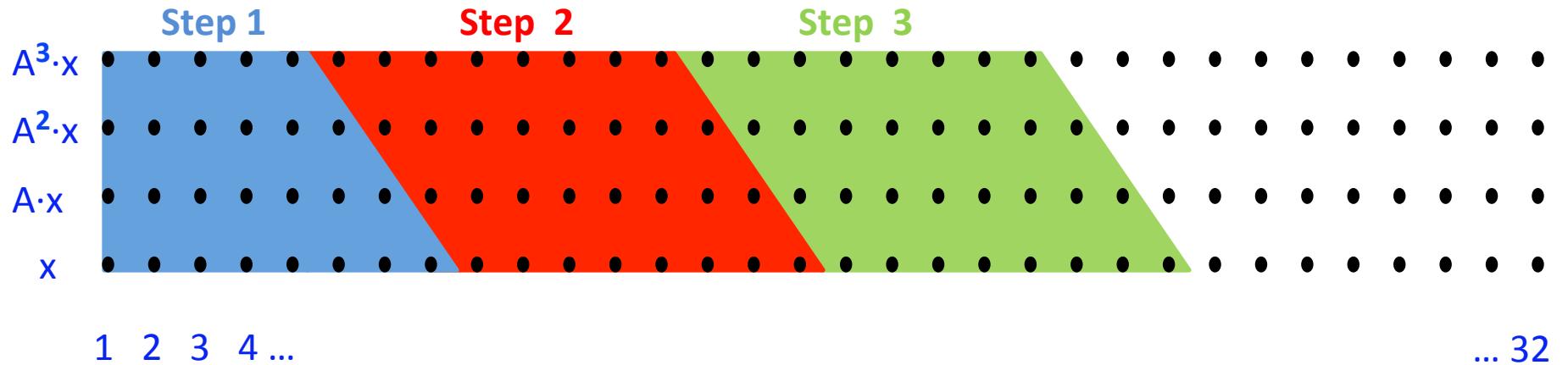


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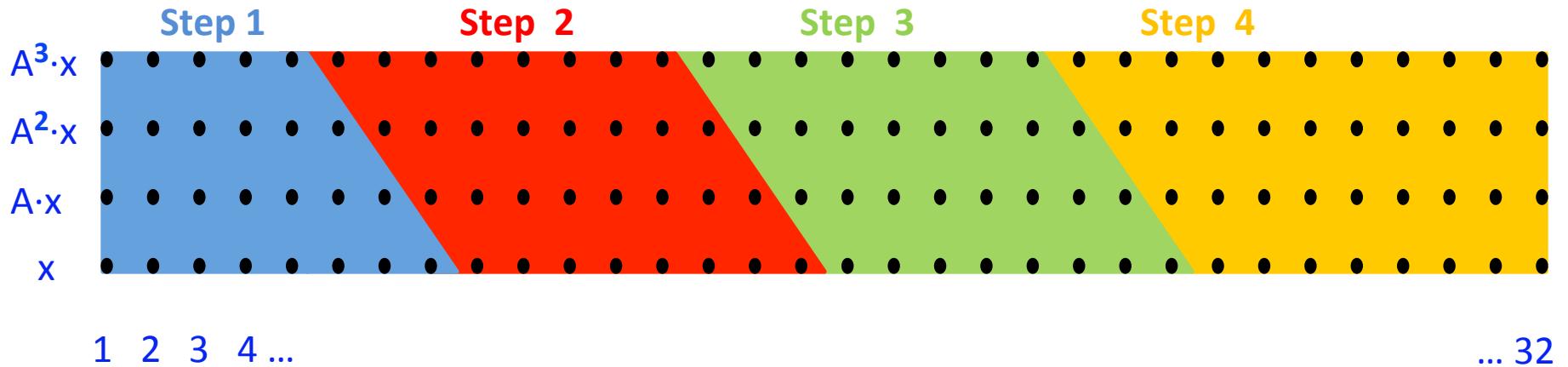


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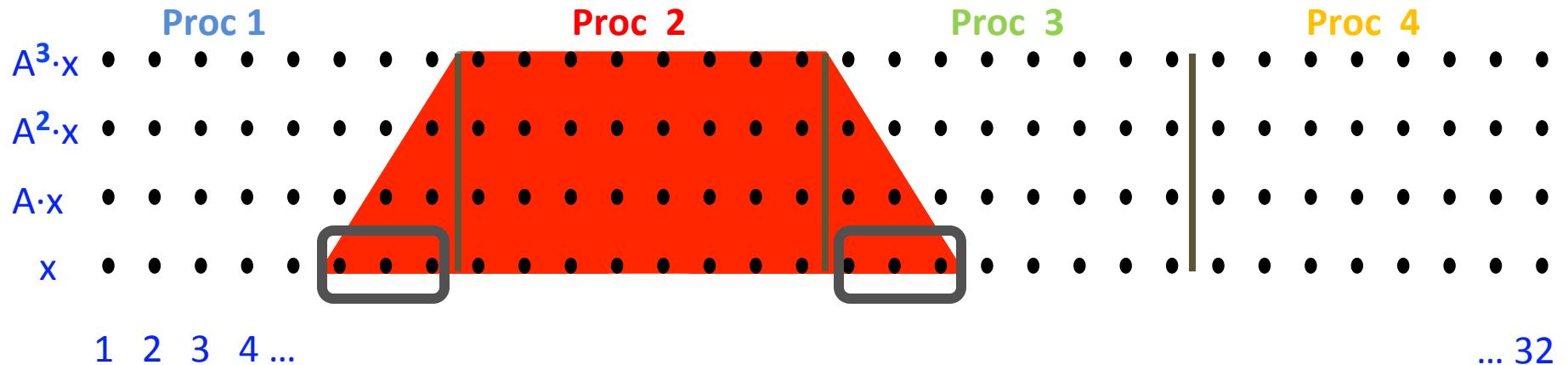
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- Example: A tridiagonal, $n=32$, $k=3$

Communication Avoiding Kernels: The Matrix Powers Kernel : $[Ax, A^2x, \dots, A^kx]$

- Replace k iterations of $y = A \cdot x$ with $[Ax, A^2x, \dots, A^kx]$
 - Parallel Algorithm

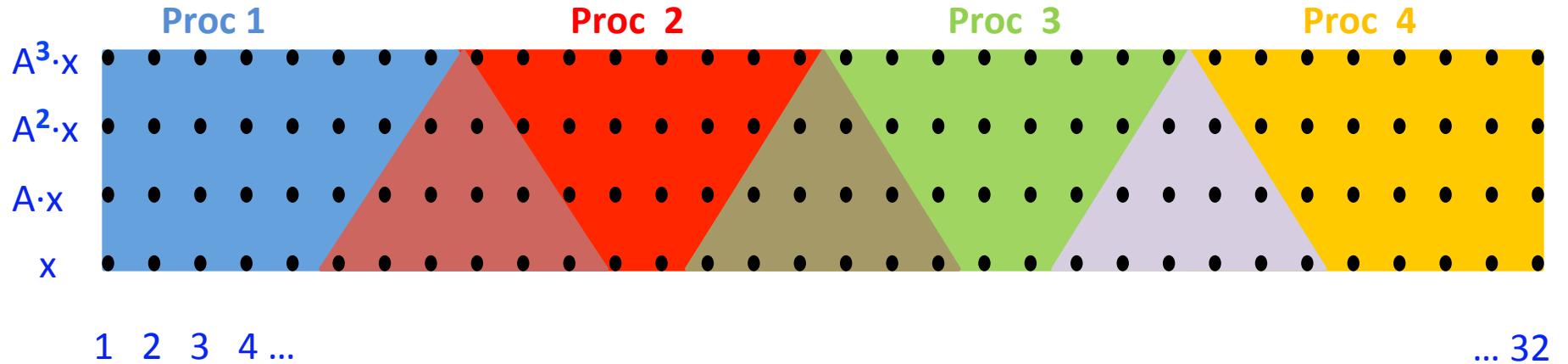


- Example: A tridiagonal, $n=32$, $k=3$
 - Each processor communicates once with neighbors

Communication Avoiding Kernels:

The Matrix Powers Kernel : $[Ax, A^2x, \dots, A^kx]$

- Replace k iterations of $y = A \cdot x$ with $[Ax, A^2x, \dots, A^kx]$
- Parallel Algorithm



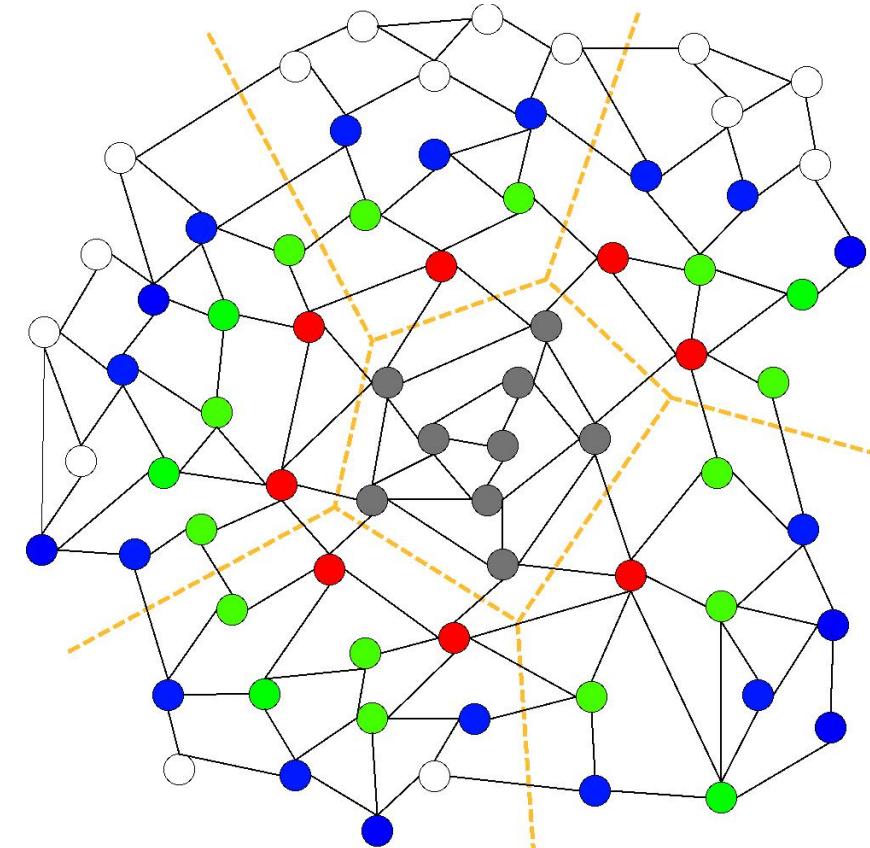
- Example: A tridiagonal, $n=32$, $k=3$
- Each processor works on (overlapping) trapezoid

Communication Avoiding Kernels: The Matrix Powers Kernel : $[Ax, A^2x, \dots, A^kx]$

Same idea works for general sparse matrices

Simple block-row partitioning →
(hyper)graph partitioning

Top-to-bottom processing →
Traveling Salesman Problem



Minimizing Communication of GMRES to solve $Ax=b$

- GMRES: find x in $\text{span}\{b, Ab, \dots, A^k b\}$ minimizing $\| Ax - b \|_2$

Standard GMRES

for $i=1$ to k

$w = A \cdot v(i-1) \dots SpMV$

$MGS(w, v(0), \dots, v(i-1))$

update $v(i)$, H

endfor

solve LSQ problem with H

Communication-avoiding GMRES

$W = [v, Av, A^2v, \dots, A^k v]$

$[Q, R] = TSQR(W)$

... “*Tall Skinny QR*”

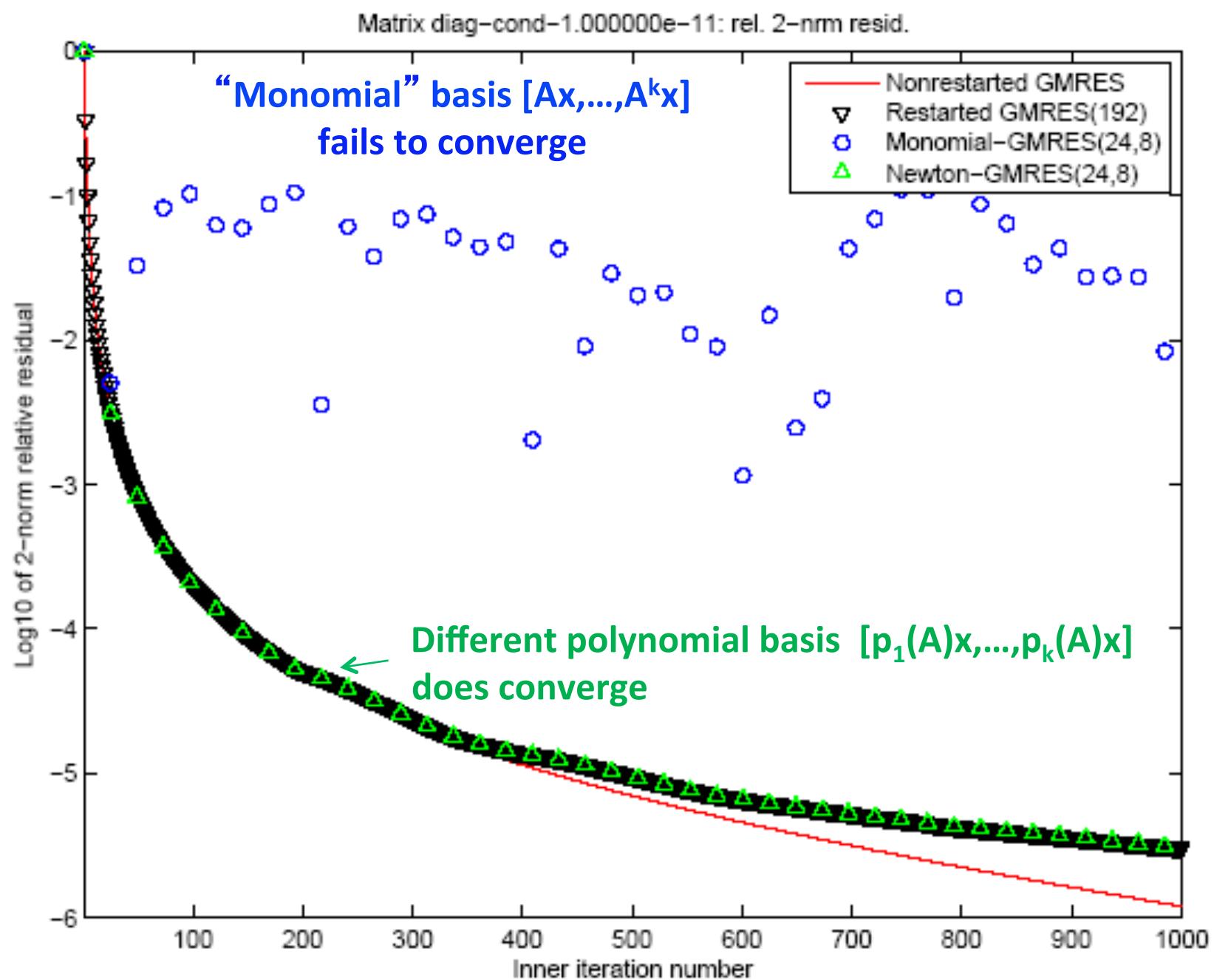
build H from R

solve LSQ problem with H

Sequential case: #words moved decreases by a factor of k

Parallel case: #messages decreases by a factor of k

- Oops – W from power method, precision lost!

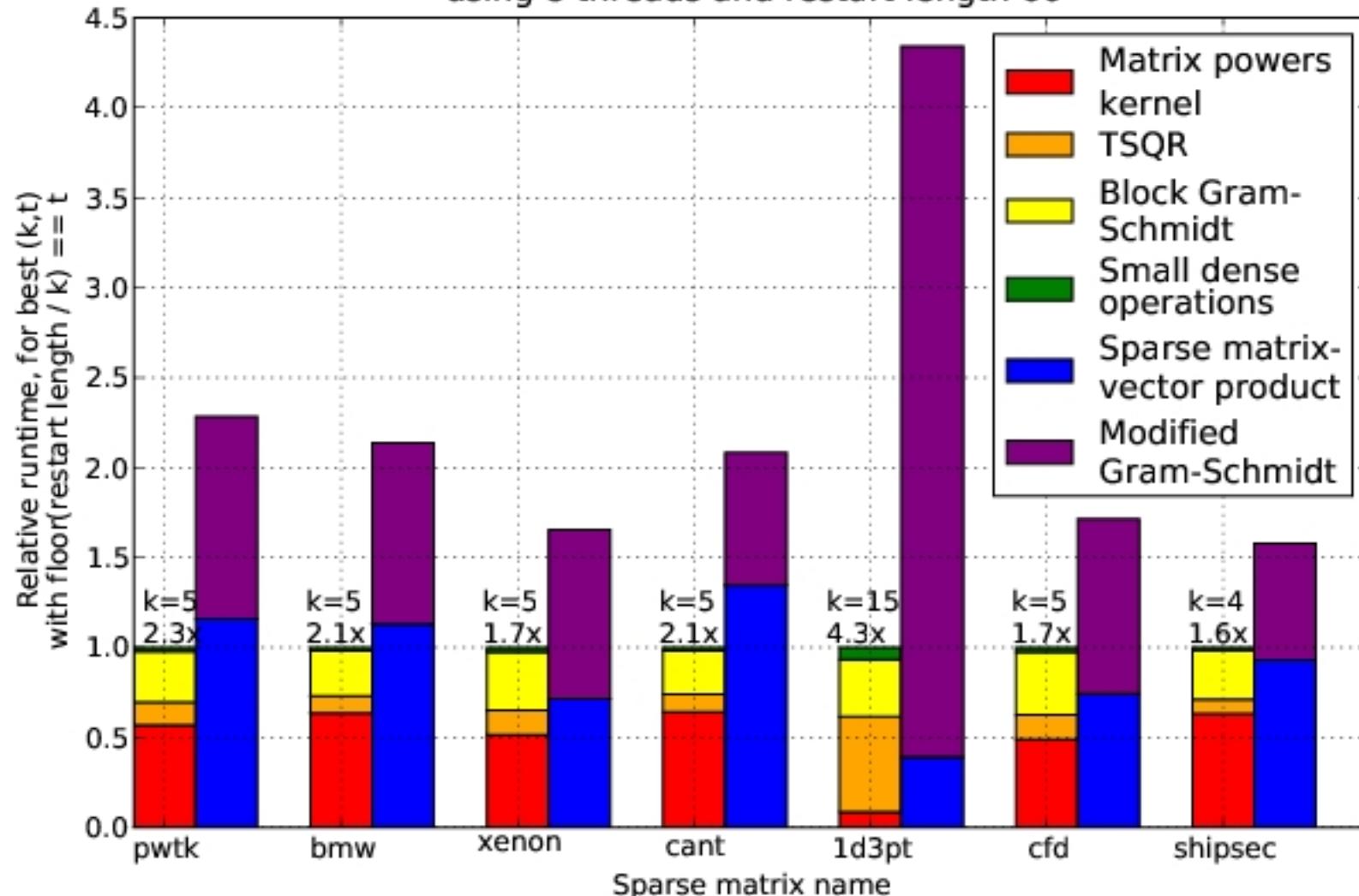


Speed ups of GMRES on 8-core Intel Clovertown

Requires Co-tuning Kernels

[MHDY09]

Runtime per kernel, relative to CA-GMRES(k,t), for all test matrices,
using 8 threads and restart length 60



Compute $r_0 = b - Ax_0$. Choose r_0^* arbitrary.

Set $p_0 = r_0$, $q_{-1} = 0_{N \times 1}$.

For $k = 0, 1, \dots$, until convergence, Do

$$\begin{aligned} P &= [p_{sk}, Ap_{sk}, \dots, A^s p_{sk}] \\ Q &= [q_{sk-1}, Aq_{sk-1}, \dots, A^s q_{sk-1}] \\ R &= [r_{sk}, Ar_{sk}, \dots, A^s r_{sk}] \end{aligned}$$

//Compute the $1 \times (3s + 3)$ Gram vector.

$$g = (r_0^*)^T [P, Q, R]$$

//Compute the $(3s + 3) \times (3s + 3)$ Gram matrix

$$G = \begin{bmatrix} P^T \\ Q^T \\ R^T \end{bmatrix} \begin{bmatrix} P & Q & R \end{bmatrix}$$

For $\ell = 0$ to s ,

$$b_{sk}^\ell = \left[B_1(:, \ell)^T, 0_{s+1}^T, 0_{s+1}^T \right]^T$$

$$c_{sk-1}^\ell = \left[0_{s+1}^T, B_2(:, \ell)^T, 0_{s+1}^T \right]^T$$

$$d_{sk}^\ell = \left[0_{s+1}^T, 0_{s+1}^T, B_3(:, \ell)^T \right]^T$$

1. Compute $r_0 := b - Ax_0$; r_0^* arbitrary;
2. $p_0 := r_0$.
3. For $j = 0, 1, \dots$, until convergence Do:
4. $\alpha_j := (r_j, r_0^*) / (Ap_j, r_0^*)$
5. $s_j := r_j - \alpha_j Ap_j$
6. $\omega_j := (As_j, s_j) / (As_j, As_j)$
7. $x_{j+1} := x_j + \alpha_j p_j + \omega_j s_j$
8. $r_{j+1} := s_j - \omega_j As_j$
9. $\beta_j := \frac{(r_{j+1}, r_0^*)}{(r_j, r_0^*)} \leftarrow \frac{\alpha_j}{\omega_j}$
10. $p_{j+1} := r_{j+1} + \beta_j(p_j - \omega_j Ap_j)$
11. EndDo

CA-BiCGStab

For $j = 0$ to $\lfloor \frac{s}{2} \rfloor - 1$, Do

$$\alpha_{sk+j} = \frac{\langle g, d_{sk+j}^0 \rangle}{\langle g, b_{sk+j}^1 \rangle}$$

$$q_{sk+j} = r_{sk+j} - \alpha_{sk+j} [P, Q, R] b_{sk+j}^1$$

For $\ell = 0$ to $s - 2j + 1$, Do

$$c_{sk+j}^\ell = d_{sk+j}^\ell - \alpha_{sk+j} b_{sk+j-1}^{\ell+1}$$

//such that $[P, Q, R] c_{sk+j}^\ell = A^\ell q_{sk+j}$

$$\omega_{sk+j} = \frac{\langle c_{sk+j+1}^1, Gc_{sk+j+1}^0 \rangle}{\langle c_{sk+j+1}^1, Gc_{sk+j+1}^1 \rangle}$$

$$x_{sk+j+1} = x_{sk+j} + \alpha_{sk+j} p_{sk+j} + \omega_{sk+j} q_{sk+j}$$

$$r_{sk+j+1} = q_{sk+j} - \omega_{sk+j} [P, Q, R] c_{sk+j+1}^1$$

For $\ell = 0$ to $s - 2j$, Do

$$d_{sk+j+1}^\ell = c_{sk+j+1}^\ell - \omega_{sk+j} c_{sk+j+1}^{\ell+1}$$

//such that $[P, Q, R] d_{sk+j+1}^\ell = A^\ell r_{sk+j+1}$

$$\beta_{sk+j} = \frac{\langle g, d_{sk+j+1}^0 \rangle}{\langle g, d_{sk+j}^0 \rangle} \times \frac{\alpha}{\omega}$$

$$p_{sk+j+1} = r_{sk+j+1} + \beta_{sk+j} p_{sk+j} - \beta_{sk+j} \omega_{sk+j} [P, Q, R] b_{sk+j}^1$$

For $\ell = 0$ to $s - 2j$, Do

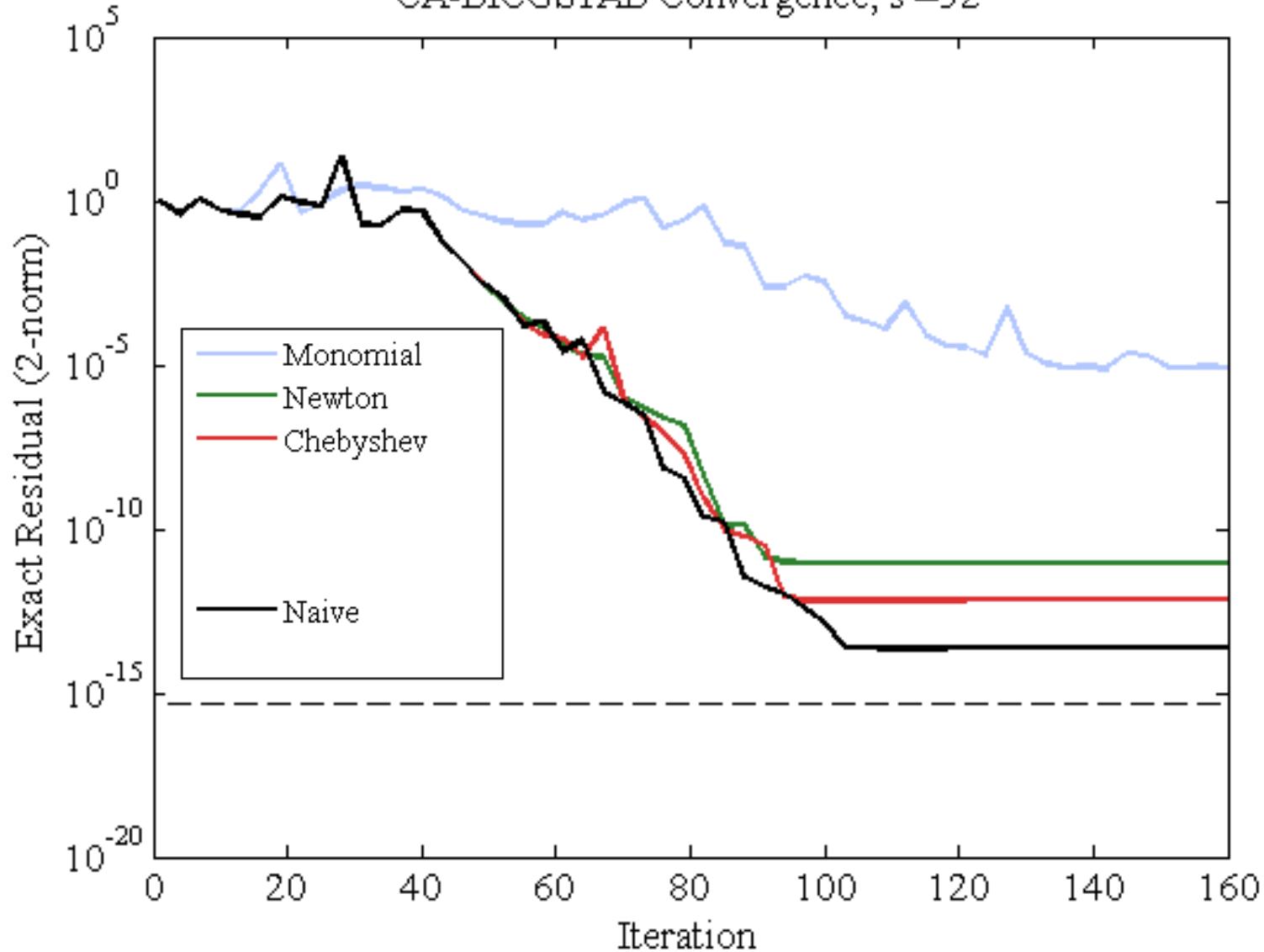
$$b_{sk+j+1}^\ell = d_{sk+j+1}^\ell + \beta_{sk+j} b_{sk+j}^\ell - \beta_{sk+j} \omega_{sk+j} b_{sk+j}^{\ell+1}$$

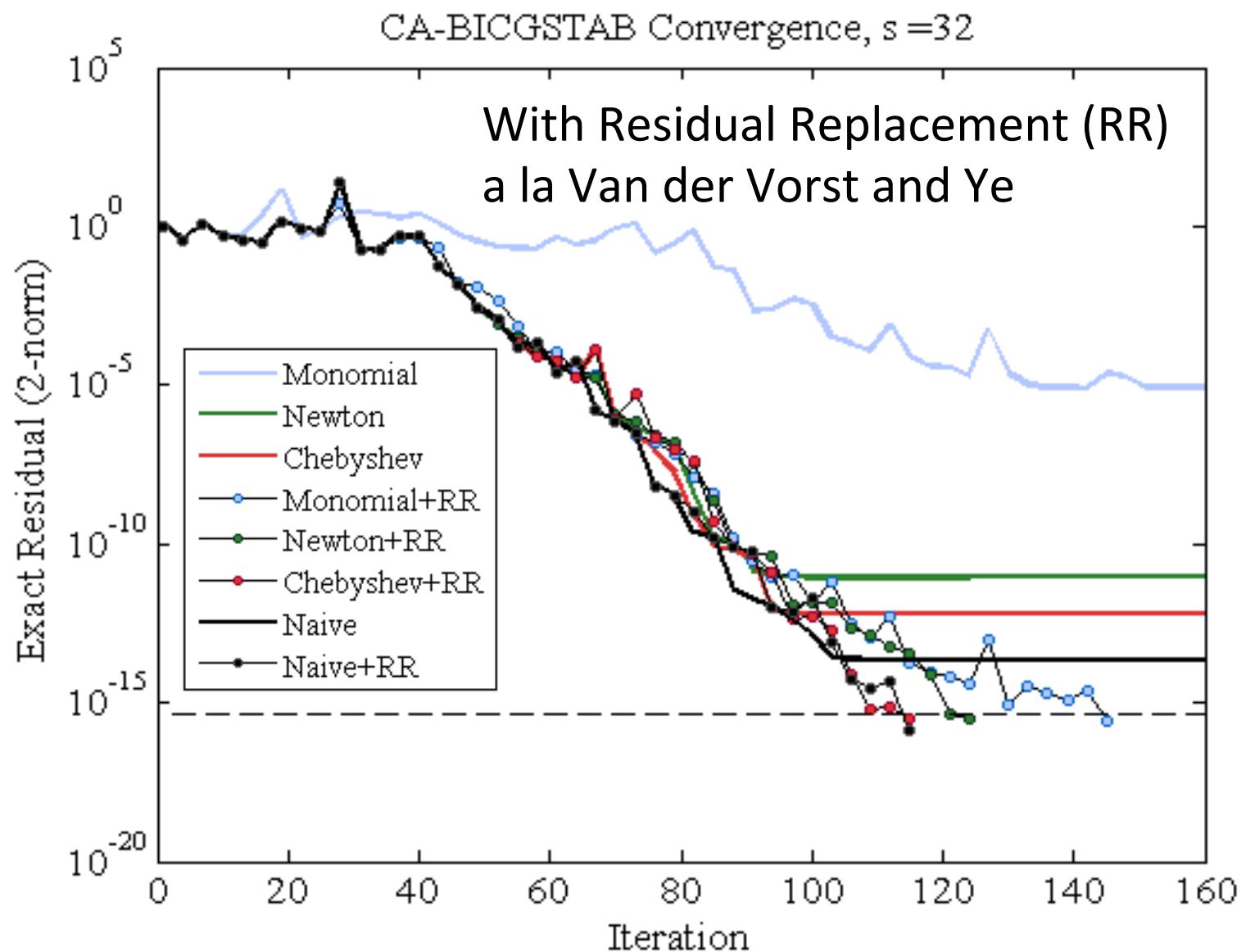
//such that $[P, Q, R] b_{sk+j+1}^\ell = A^\ell p_{sk+j+1}$.

EndDo

EndDo

CA-BICGSTAB Convergence, s = 32





	Naive	Monomial	Newton	Chebyshev
Replacement Its.	74 (1)	[7, 15, 24, 31, ..., 92, 97, 103] (17)	[67, 98] (2)	68 (1)

Summary of Iterative Linear Algebra

- New lower bounds, optimal algorithms, big speedups in theory and practice
- Lots of other progress, open problems
 - Many different algorithms reorganized
 - More underway, more to be done
 - Need to recognize stable variants more easily
 - Preconditioning
 - Hierarchically Semiseparable Matrices
 - Autotuning and synthesis
 - Different kinds of “sparse matrices”

For more details

- Bebop.cs.berkeley.edu
- CS267 – Berkeley’s Parallel Computing Course
 - Live broadcast in Spring 2013
 - www.cs.berkeley.edu/~demmel
 - All slides, video available
 - Prerecorded version broadcast in Spring 2013
 - www.xsede.org
 - Free supercomputer accounts to do homework
 - Free autograding of homework

Collaborators and Supporters

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- bebop.cs.berkeley.edu

Summary

Time to redesign all linear algebra, n-body, ...
algorithms and software
(and compilers)

Don't Communic...